ANL-76-11 Rev. 1

ANL-76-11 Rev. 1

PTOLEMY

A Program for Heavy-ion Direct-reaction Calculations

by

M. H. Macfarlane and Steven C. Pieper

U of C-AUA-USDOE

ARGONNE NATIONAL LABORATORY, ARGONNE, ILLINOIS

Prepared for the U. S. DEPARTMENT OF ENERGY
under Contract W-31-109-Eng-38

Printed in the United States of America
Available from
National Technical Information Service
U. S. Department of Commerce
5285 Port Royal Road
Springfield, Virginia 22161
Price: Printed Copy $6.50; Microfiche $3.00

ANL-76-11 Rev. 1
Mathematics and
Computers
(UC-32)

Argonne National Laboratory
9700 South Cass Avenue
Argonne, Illinois 60439

P T O L E M Y

A Program for Heavy-ion Direct-reaction Calculations

M. H. Macfarlane and Steven C. Pieper

Physics Division

Sophisticated programs contain subtle errors.

April 1978

This manual corresponds to the March, 1978, version of Ptolemy. Many important additions and improvements have been made to Ptolemy since the previously-documented version of February 1976. An indication of this is that the list of keywords has been expanded by thirty. Collective-model inelastic excitation has been added. The computation of the transfer DWBA amplitudes has been significantly improved by the use of interpolation in the Ri+Ro variable. Elastic scattering and reactions involving identical particles may now be computed. Simultaneous optical model fits to several different elastic channels are possible. Significant changes to this manual are marked with a vertical bar (|) in the left margin and should be carefully reviewed. In addition the contents of the manual have been extensively re-ordered.

Ptolemy is still under development and it may be expected that some of the specifications given in this manual will change from time to time without warning.

Contents

ABSTRACT

Ptolemy is an IBM/360 program for the computation of nuclear elastic and direct-reaction cross sections. It carries out optical-model fits to elastic-scattering data at one or more energies and for one or more combinations of projectile and target, collective model DWBA calculations of excitation processes, and finite-range DWBA calculations of nucleon-transfer reactions. It is fast and does not require large amounts of core. The input is exceptionally flexable and easy to use. This report outlines the types of calculations that Ptolemy can carry out, summarizes the formulas used, and gives a detailed descripton of its input.

I - Introduction

Ptolemy is a program for fitting optical-model potentials to elastic scattering data, and for the computation of the Distorted Wave Born Approximation to nuclear direct-reaction amplitudes. Either the collective-model DWBA for inelastic excitation or the finite-range DWBA for transfer reactions may be computed. No use is made of approximations that rely on the short range of nuclear interactions (e.g. zero-range and no-recoil approximations). Ptolemy is specifically designed for heavy ion reactions but is nonetheless very efficient for light ion reactions. Advantages of Ptolemy over other DWBA codes include high speed, low core requirements, and ease of use.

Ptolemy derives its speed and compactness from several design features:

1) Substantial effort has been put into the development of the subroutine that picks the three-dimensional integration grid that is used in the DWBA transfer calculations. This subroutine makes use of the bound state form factor and the properties of the scattering wavefunctions. This efficiently chosen integration grid results in the need for relatively small numbers of integration points; as an example, a grid consisting of 24 X 10 X 10 points will give accuracies of 1 or 2 percent for many heavy-ion reactions at moderate energies.

2) In high-energy heavy-ion DWBA transfer calculations, the scattering waves oscillate rapidly while the form factor varies slowly. However the computation of the form factor is the most time consuming aspect of the calculation. Therefore the form factor is computed on a coarse grid and interpolated to the finer grid needed for the integrals involving the scattering waves. This interpolation results in a reduction in the total computer time by a factor of two to five in typical heavy-ion calculations.

3) Interpolation and extrapolation in L-space is used to reduce the number of radial integrals that must be computed. Interpolation is achieved by fitting a continued fraction to the computed values, while the exponential form of the radial integrals for large L is used for extrapolation. For Oxygen on Lead reactions, a time savings of 80% is realized by this method.

4) The two inner loops of the radial integral computation for transfer reactions have been coded in assembly language that is specifically designed for the special features of the 370/195. These loops function some three times faster than the equivalent Fortran-generated code.

5) The calculation of the angular transforms in transfer reactions has been implemented using cosines instead of spherical

harmonics. This approach avoids the large numerical cancellations that occur in the more conventional Legendre decomposition methods if the exchanged orbital angular momentum is relativly large. A specially designed in-line cosine routine and iterative evaluations of cosines are used to reduce the cosine computation time.

6) The Coulomb terms of the inelastic excitation amplitudes are computed using recursion relations in L. The starting values for the recursion relations are generated using Belling's asymptotic expansion for integrals of Coulomb wavefunctions and powers of r. A new asymptotic expansion of Coulomb wavefunctions for large argument is used in these calculations. The result of these techniques is a high speed program for the Coulomb excitation in which it is not necessary to be concerned with either orbital angular momentum or radial cut-offs.

7) The optical-model potential fitting part of Ptolemy uses state-of-the-art minimization routines that make specific use of the sum of squares property of the function (chi-squared) being minimized. The gradients required by these minimizers are computed analytically.

8) The computation of the transfer amplitudes has been factored into segments in such a way that the recomputation of the same quantities is held to a reasonable (although not absolute) minimum without the need for extremely large tables. Scratch files are not used in any part of the program.

9) Ptolemy has been overlaid to about 18% of its unoverlaid size. Nonetheless, overlay thrashing is not excessive and is independent of the size of the calculation. The overlay processing adds an estimated three seconds to a complete calculation.

10) All arrays used in a Ptolemy calculation are stored in a section of core referred to as the allocator. This allocator is obtained at the start of the job from the available core in the region specified on the user's JOB card. Space in the allocator is reused when the data contained in it is no longer needed. Since the allocator size can change from job to job, small calculations may be carried out in small regions while larger calculations are possible without the recompilation of any part of Ptolemy.

The result of these and other features is a very fast program for the finite-range DWBA. The ^{208}Pb(^{16}O,^{15}N)^{209}Bi(7/2$^-$) reaction including both L transfers at 104 MeV requires only 17 seconds (on the IBM 370/195) and 220K of core. Further time savings may be realized by storing the form factor integrals in a dataset for use in subsequent calculations with different optical potentials. Most inelastic excitation calculations require less than one minute of 370/195 cpu time.

In addition to its great speed, Ptolemy provides the user with an especially simple form of input. The input is designed to be flexible, tolerant of minor syntactical variations, concise and easy to remember. Extensive checking of the input is carried out in an effort to allow the same problem to be stated in a variety of ways and to eliminate the chance of calculations being made with undefined or otherwise unexpected parameters. In the following sections it will become evident that many quantities may be defined in more than one way. Often there will be the possibility of a direct specification of a parameter that can also be determined by Ptolemy from other input. In most cases if the user explicitly specifies the value, Ptolemy will not use the indirectly specified value nor will it check the two values for consistency. Therefore one should avoid needless duplication of input so that inadvertant inconsistencies do not occur. An example would be the specification of Q after the bound state calculations — the new value of Q would be used in determining the outgoing state scattering energy even though it might be inconsistent with the difference of the bound state energies. (In this case a warning message would be printed.)

Provision is made for keeping final results (radial integrals, elastic S-matrix elements, differential cross sections, etc.) in a form suitable for subsequent processing with Speakeasy+. This is particularly useful for the production of graphs showing the results of one or more DWBA calculations. In addition one may use the extensive facilities of Speakeasy to manipulate cross sections or radial integrals interactively.

In addition to the computation of DWBA cross sections, Ptolemy can also be used to fit optical potentials to elastic scattering data. The specification of the parameters to be varied is both simple and flexable; the user does not need to write a subroutine for each fit to be made. The method of entering data is quite general; if the user's data is already punched on cards for a different fitter, he will probably not need to repunch it for Ptolemy. Fits to data at several energies may be made, and several keywords are provided to give the optical potential a dependance on the scattering energy. The user is given a choice of six different minimum-search programs including four that use analytically computed gradients. Two of the latter fitters work exceptionally well and 12-parameter fits to $^{16}O+^{208}Pb$ data at five different energies may be made in less than a minute of /195 time.

In the next section we present the formulas used in Ptolemy. The syntax used in Ptolemy's input is described in Sec. III. Sec. IV describes elastic-scattering and bound-state calculations and contains basic material (such as potential definitions) that is used in the subsequent sections. The next three sections (V, VI, and VII) discuss optical model fits, inelastic excitation, and

---

+ S. Cohen and S. C. Pieper, "The Speakeasy-3 Reference Manual," Argonne National Laboratory Report ANL-8000 (1977).

transfer reactions respectively. These three sections are largely independant of each other; where necessary cross references are made. Section VIII presents some of the control keywords that perform functions auxilary to the calculational functions. Appendix A contains a complete list of Ptolemy keywords and their default values. Appendix B provides core and run time estimates. Appendix C shows the JCL needed to use Ptolemy and Appendix D contains the complete input decks for some sample jobs.

This manual does not enumerate all possible variants and interpretations of the Ptolemy input; rather it is limited to the most straightforward methods of stating the problem to be solved. For many DWBA calculations and optical-model fits, the necessary input can be inferred directly from the examples given in Appendix D, to which the tyro is referred. The only aspect of the input that is not clear upon inspection of these examples is the use of the PARAMETERSET keyword which is discussed on page 40.

II - Summary of Formulas

This chapter contains a summary of the formulas used in Ptolemy for evaluating elastic, inelastic and transfer cross sections. Since all of the formulas are standard, no attempt is made to present deriviations.

A - Two-body Channels

We will consider two particles (nuclei) referred to as the "projectile" (subscript p) and the "target" (subscript t). For scattering states these designations will have their customary meanings, while for bound states the only distinction is that the spin of the projectile determines the spin-orbit force. The reduced mass is

$$M = \frac{M_p M_t}{M_p + M_t} \mathcal{M} \qquad \text{(II.1)}$$

where M_p and M_t are the atomic weights of the two nuclei and $\mathcal{M}$ is the atomic mass unit [Eq. (II.100)].

1. Bound States

The Schrödinger equation for bound states may be written as

$$\left[-\frac{1}{r^2}\frac{d}{dr} r^2 \frac{d}{dr} + \frac{\ell(\ell+1)}{r^2} + \frac{2M}{\hbar^2} V(r) + \kappa^2\right] \phi(r) = 0, \qquad \text{(II.2)}$$

$$\kappa = \sqrt{-2 M E} / \hbar \qquad \text{(II.3)}$$

and E is the (negative) energy of the bound state. For large r, $\phi(r)$ tends to a Whittaker function:[1]

$$\phi(r) \xrightarrow[r\to\infty]{} \frac{N}{r} W_{-\eta,\ell+\frac{1}{2}}(2 \kappa r) , \qquad \text{(II.4)}$$

where N is a normalization constant and η is the Sommerfeld parameter for the bound state:

$$\eta = Z_p Z_t \alpha M c / (\hbar \kappa) . \qquad \text{(II.5)}$$

The relevant combinations of the fine-structure constant α, the speed of light c, and the Planck constant $\hbar$ are given in Eqs. (II.99) - (II.101). The bound-state wave function is real and normalized such that

$$\int_0^\infty dr\, r^2\, [\phi(r)]^2 = 1 \quad . \tag{II.6}$$

The sign of $\phi(r)$ follows the conventions of Meyer and Jensen[2], namely $\phi(r)$ is positive for small r.

2. Scattering States

The Schrödinger equation for scattering states is written as

$$[- \frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + \frac{2\,M}{\hbar^2}\, V(r) - k^2]\, f_\ell(r) \ , \tag{II.7}$$

where the wave number is

$$k = \sqrt{2\,M\,E}\,/\hbar \tag{II.8}$$

with E the center-of-mass scattering energy. If the potential contains a spin-orbit component, the f_ℓ should also contain a label for the total projectile angular momentum; we will for the moment suppress this label. The scattering wavefunctions are normalized such that

$$f_\ell(r) \underset{r\to\infty}{\longrightarrow} \tfrac{1}{2}[(1 + S_\ell)F_\ell(\eta,kr) + i\,(1-S_\ell)G_\ell(\eta,kr)] \ , \tag{II.9}$$

where F_ℓ and G_ℓ are the regular and irregular Coulomb wavefunctions[1] and η is the Sommerfeld parameter:

$$\eta = Z_p\, Z_t\, \alpha\, M\, c/(\hbar\, k), \tag{II.10}$$

$$= Z_p\, Z_t\, \alpha \sqrt{\frac{M\,c^2}{2\,E}} \quad . \tag{II.11}$$

The elastic scattering S-matrix element S_ℓ is defined by Eq. (II.9).

If there are no spin-dependent forces and if the particles are not identical, the elastic scattering cross section is given by

$$\frac{d\sigma}{d\Omega} = |F\,(\theta)|^2 \quad . \tag{II.12}$$

If the particles are identical, but there are no spin-dependent forces, the cross section is

$$\frac{d\sigma}{d\Omega} = |F^{\pm}(\theta)|^2 \mp \frac{S_p}{S_p+\frac{1}{2}} [|F^{+}(\theta)|^2 - |F^{-}(\theta)|^2] \tag{II.13}$$

where the upper signs are for Bose statistics and the lower signs are for Fermi statistics. Here S_p is the spin of the particles. Finally, for a spin-½ projectile interacting with a spinless target via a spin-orbit force, the spin-averaged cross section is

$$\frac{d\sigma}{d\Omega} = |F(\theta)|^2 + |B(\theta)|^2 \quad . \tag{II.14}$$

We do not consider more complicated systems with spin-dependent forces.

The amplitudes in the above equations are sums of Rutherford and nuclear components,

$$F(\theta) = F_R(\theta) + F_N(\theta) \quad , \tag{II.15}$$

$$F_R(\theta) = -\frac{\eta}{2k[\sin\frac{1}{2}\theta]^2} \, e^{2i[\sigma_\ell - \eta \ln \sin\frac{1}{2}\theta]} \quad , \tag{II.16}$$

$$F_N(\theta) = \frac{1}{2ik\,(2S_p+1)} \sum_{\ell,j} (2j+1)\,(S_{\ell,j}-1)\, e^{2i\sigma_\ell} P_{\ell,0}(\cos\theta) \quad , \tag{II.17}$$

$$F^{\pm}(\theta) = F(\theta) \pm F(\pi-\theta) \quad , \tag{II.18}$$

and

$$B(\theta) = \frac{1}{2ik} \sum_{\ell} [S_{\ell,\ell+\frac{1}{2}} - S_{\ell,\ell-\frac{1}{2}}]\, e^{2i\sigma_\ell} P_{\ell,1}(\cos\theta) \quad . \tag{II.19}$$

Here S_p is the spin of the projectile and the S-matrix elements have been labeled with both ℓ and j to allow for a spin-orbit interaction. If there is no spin-orbit force, one has

$$\frac{1}{2S_p+1} \sum_j (2j+1)\, S_{\ell,j} = (2\ell+1) S_\ell \quad . \tag{II.20}$$

The Coulomb phase shifts are

$$\sigma_\ell = \operatorname{Arg} \Gamma\,(\ell+1+i\eta) \quad , \tag{II.21}$$

and the conventions of Ref. 1 are used for the Legendre functions $P_{\ell,m}$. In the Rutherford amplitude (II.16) an alternative form is given by the replacement

$$\frac{\eta}{2k} = Z_p Z_t \alpha \hbar c/(4E) \quad . \tag{II.22}$$

The total reaction cross sections are given by

$$\sigma_{Reac} = \frac{\pi}{k^2(2 S_p+1)} \sum_{\ell,j} (2j+1) (1-|S_{\ell,j}|^2) \tag{II.23}$$

for non-identical particles and by

$$\sigma_{Reac} = \frac{2\pi}{k^2(2 S_p+1)} \left\{ S_p \sum_{\ell} (2\ell+1) (1-|S_\ell|^2) + \sum_{\substack{\ell \text{ even} \\ \text{or odd}}} (2\ell+1) (1-|S_\ell|^2) \right\} \tag{II.24}$$

for identical particles. Here the second sum is over even partial waves for Bose statistics and over odd partial waves for Fermi statistics.

One can define a "nuclear total cross section"

$$\sigma_{Nuc} = \frac{4\pi}{k} \text{ Im } F_N(0) \tag{II.25}$$

for non-identical particles, and

$$\sigma_{Nuc} = \frac{4\pi}{k(2 S_p+1)} [2 S_p \text{ Im } F_N(0) + \text{Im } F_N^{\pm}(0)] \tag{II.26}$$

for identical particles. If there is no Coulomb force, these quantities are just the total cross sections:

$$\sigma_{Nuc} = \sigma_{el} + \sigma_{Reac} \tag{II.27}$$

where σ_{el} is the integral over angles of the elastic cross section. Schwarzschild et. al.[3] have discussed the significance of σ_{Nuc} in the presence of a Coulomb force; for heavy-ion scattering σ_{Nuc} is usually quite small.

B - Inelastic Excitation

We consider the inelastic excitation process

$$A(a,b)\,B \tag{II.28}$$

with either

$$b = a \qquad B = A^* \tag{II.29}$$

for target excitation or

$$b = a^* \qquad B = A \tag{II.30}$$

for projectile excitation.

The outgoing kinetic energy in the c.m. system is

$$E_{out} = E_i + Q \tag{II.31}$$

where E_i is the incoming c.m. energy and the Q value is given by

$$Q = E_A + E_a - E_B - E_b \tag{II.32}$$

where the E_k are the total energies (in MeV) of the nuclear states involved:

$$E_k = (Z_k M_p + N_k M_n)c^2 + (M_{xc})_k + E^*_k \quad , \tag{II.33}$$

or

$$E_k = E_g\,(Z_k, N_k) + E^*_k \quad . \tag{II.34}$$

Z_k, N_k are the numbers of nucleons in the nuclear state k, $(M_{xc})_k$ is the ground-state mass excess of the nucleus with Z_k protons and N_k neutrons and E^*_k is the excitation energy if state k is excited. $E_g(Z_k, N_k)$ is the total ground-state energy (or mass × c^2) of the nucleus (Z_k, N_k).

Ptolemy evaluates the inelastic cross sections in DWBA using collective-model form factors for the nuclear part of the excitation. The distorted waves are the solution of Eq. (II.7) with the normalization of Eq. (II.9). These distorted waves must, of course, be separately evaluated in the incoming [a+A] and outgoing [b+B] channels.

1. Differential Cross Section

The differential cross section at a c.m. scattering angle θ for the excitation process is written as

$$\frac{d\sigma}{d\Omega} = \frac{1}{E_i\, E_{out}} \frac{k_{out}}{k_i} \; R \sum_{L_x M_x} \left| G_{M_x}^{L_x} (\theta) \right|^2 , \tag{II.35}$$

where R is a spin-statistical factor:

$$R = \frac{2J_b + 1}{2J_a + 1} \qquad \text{(projectile excitation)},$$

$$= \frac{2J_B + 1}{2J_A + 1} \qquad \text{(target excitation)} \; . \tag{II.36}$$

Here k_i and k_{out} are the wave numbers (Eq. II.8) in the incoming and outgoing channels and J_a, J_b, J_A and J_B are the intrinsic angular momenta of the four nuclei. The multipolarity of the transition is labeled by L_x.

The multipole transition amplitude may be decomposed into a term reflecting the amount of deformation and a geometric term:

$$G_{M_x}^{L_x} (\theta) = A_{L_x} \; B_{M_x}^{L_x} (\theta) \quad . \tag{II.37}$$

2. Geometrical Component and Effective Interactions

The "geometrical" component is

$$B_{M_x}^{L_x} = \sqrt{4\pi}\; i^{L_x} \sum_{L_i\, L_{out}} C_{M_x, -M_x, 0}^{L_{out}, L_x, L_i}$$

$$\times \; I_{L_i, L_{out}, L_x} \; Y_{-M_x}^{L_{out}} (\theta, 0) \; , \tag{II.38}$$

where $Y_M^L(\theta,\phi)$ is a spherical harmonic and $C_{M_1,M_2,M}^{L_1,L_2,L}$ is a Clebsch-Gordan coefficient, both defined according to Condon-Shortley conventions.

The radial integrals are given by

$$I_{L_i, L_{out}, L_x} = \sqrt{\frac{2\, L_{out} + 1}{4\pi}} \; \left| C_{0,\,0,\,0}^{L_{out}, L_x, L_i} \right| \; e^{i(\sigma_i + \sigma_{out})}$$

$$\times \int_0^\infty f_{L_i}(r)\; \mathcal{H}_{L_x}(r)\; f_{L_{out}}(r) \quad dr \quad . \tag{II.39}$$

The symbols σ_i and σ_{out} designate the Coulomb phase shifts $\sigma_{L_i}(\eta_i)$ and $\sigma_{L_{out}}(\eta_{out})$ respectively. The effective interaction H contains both nuclear and electric Coulomb contributions:

$$H_{L_x}(r) = H_{L_x,N}(r) + H_{L_x,C}(r) \quad . \tag{II.40}$$

The nuclear component of the effective interaction is

$$H_{L_x,N}(r) = - \frac{\beta_{L_x}}{\overline{\beta}_{L_x}} \left[R' \frac{d\,V(r)}{dr} + iR'_I \frac{d\,V_I(r)}{dr}\right] \quad . \tag{II.41}$$

where V and V_I are the real and imaginary parts of an optical potential. The radii R' and R'_I are the radii of the excited nucleus; specifically,

$$R' = r_0\, A'^{1/3} \quad ,$$
$$R'_I = r_{I0}\, A'^{1/3} \quad , \tag{II.42}$$

where A' = A for target excitation, A' = a for projectile excitation. The nuclear deformation parameter is β_{L_x} so that $R'\beta_{L_x}$ and $R'_I\,\beta_{L_x}$ are the deformation lengths. We have normalized the effective interaction to the average of the nuclear and Coulomb deformation parameters:

$$\overline{\beta}_{L_x} = \tfrac{1}{2}\,(\beta_{L_x} + \beta_{L_x,C}) \quad . \tag{II.43}$$

The Coulomb part of the effective interaction is derived from the multipole expansion of the potential between a point charge and a uniformly charged sphere.

$$H_{L_x,C}(r) = \frac{\beta_{L_x,C}}{\overline{\beta}}\; R'_C\; \frac{3Z_aZ_Ae^2}{2L_x+1} \begin{cases} \dfrac{r^{L_x}}{R_C^{L_x+2}} & r < R_C \quad , \\[2ex] \dfrac{R_C^{L_x-1}}{r^{L_x+1}} & r > R_C \quad , \end{cases} \tag{II.44}$$

where Z_a and Z_A are the atomic numbers of the two nuclei. Note the distinction between the Coulomb radius of the excited nucleus:

$$R'_C = r_{C0}\, A'^{1/3} \tag{II.45}$$

and the Coulomb radius of the optical potential:

$$R_C = r_{C0}\, (a^{1/3} + A^{1/3}) \quad . \tag{II.46}$$

The Coulomb deformation parameter $\beta_{L_x,C}$ is related to the reduced transition rate $B(E,L_x,\uparrow)$ by

$$\begin{aligned} B(E,L_x,\uparrow) &= \frac{2J_{final}+1}{2J_{initial}+1}\; B(E,L_x,\downarrow) \quad , \\ &= \left[\frac{3Z}{4\pi}\;\; \frac{R'^{\,L_x}_C}{10}\;\; \beta_{L_x,C}\right]^2 \times \frac{(2J_{final}+1)}{(2J_{initial}+1)(2L_x+1)} \end{aligned} \tag{II.47}$$

where $B(E,L_x,\uparrow)$ is given in units of e^2 barn^{L_x} and R'_C is in fm. The $\beta_{L_x,C}$ so defined can be related to a nuclear deformation only for 0^+ ground states; however Ptolemy correctly computes the Coulomb excitation from other ground states if the $B(E,L_x,\uparrow)$ is given.

3. Strength of Effective Interaction

The strength constant in Eq. (II.37) is given by

$$A_{L_x} = \bar{\beta}_{L_x} \,/\, \sqrt{2L_x+1} \quad , \tag{II.48}$$

where $\bar{\beta}_{L_x}$ is defined in Eq. (II.43).

C - Transfer Reactions

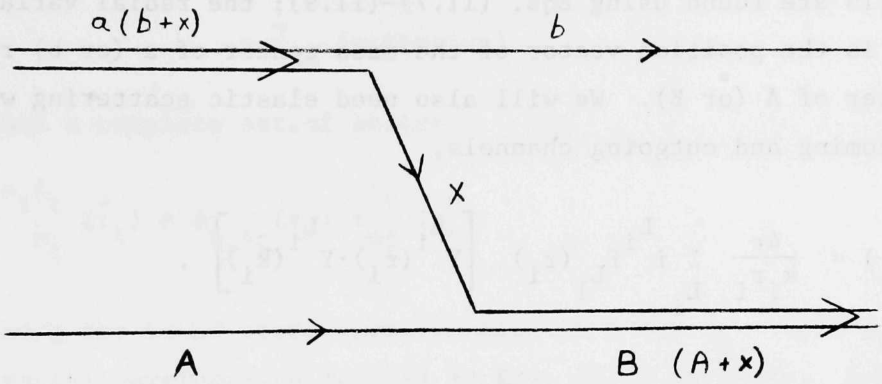
Ptolemy computes amplitudes and cross sections of nucleon-transfer reactions

$$A\ (a,b)\ B \tag{II.49}$$

using the full distorted-wave Born approximation[4] (DWBA), without further approximations based on the short range of nuclear interactions. In the incoming channel (A,a), A is the target and a is the projectile; in the outgoing channel (B,b), B is the residual nucleus and b the ejectile. A, a, B, b will be used both as identifiers of the nuclear states involved and as symbols for the total numbers of nucleons. The group of nucleons transferred (or the number of transferred nucleons) will be denoted by x.

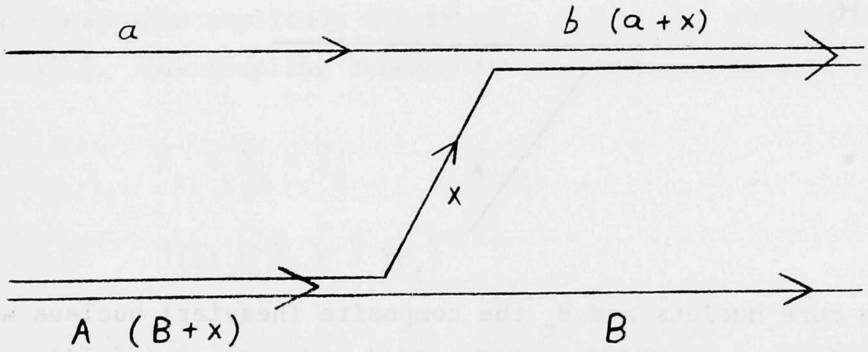
1. Possible Reactions

(i) If a > b, the reaction (II.49) is a stripping reaction.



$$a = b + x \qquad \text{(stripping)}$$
$$B = A + x \tag{II.50}$$

(ii) If a < b, the reaction (II.49) is a pick-up reaction.



$$b = a + x \qquad \text{(pick-up)}$$
$$A = B + x \tag{II.51}$$

2. Two-Body States

Calculation of the transfer cross sections involves the combination of four elements—the scattering wave functions in incoming (i) and outgoing (out) channels and bound-state wave functions representing the composite nucleus at each reaction vertex. The vertex involving A, B and x will be referred to as the target vertex and the corresponding bound state as the target bound state; the vertex involving a, b and x will be referred to as the projectile vertex and the corresponding bound state the projectile bound state.

The kinetic energies in the incoming and outgoing channels are related by Eqs. (II.31)-(II.34) and the elastic scattering distorted waves for these two channels are found using Eqs. (II.7)-(II.9); the radial variable in these equations is the position vector of the mass center of a (or b) relative to the mass center of A (or B). We will also need elastic scattering wave-functions in incoming and outgoing channels,

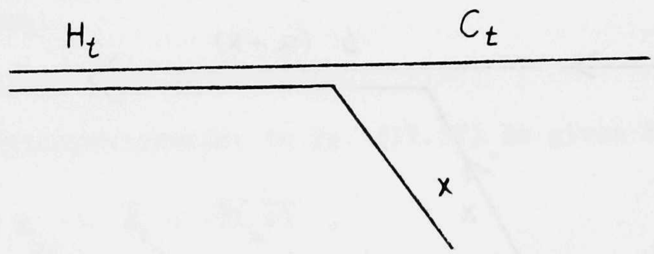
$$\chi^{+}(\vec{k}_i, \vec{r}_i) = \frac{4\pi}{k_i r_i} \sum_{L_i} i^{L_i} f_{L_1}(r_i) \left[Y^{L_i}(\hat{r}_i) \cdot Y^{L_i}(\hat{k}_i) \right] , \tag{II.52}$$

and

$$[\chi^{-}(\vec{k}_{out}, \vec{r}_{out})]^{*} = \frac{4\pi}{k_{out} r_{out}} \sum_{L_{out}} i^{L_{out}} f_{L_{out}} \left[Y^{L_{out}}(\hat{r}_{out}) \cdot Y^{L_{out}}(\hat{k}_{out}) \right] . \tag{II.53}$$

Consider next the interaction vertices.

(i) <u>The Target Vertex: $t = (x, C_t)$</u>



Let C_t denote the core nucleus and H_t the composite (heavier) nucleus at the target vertex

$$\begin{aligned} C_t &= B \text{ (pick-up)} & H_t &= A \text{ (pick-up)} \\ &= A \text{ (stripping)} & &= B \text{ (stripping)} \end{aligned} \quad . \tag{II.54}$$

In either case vertex t is regarded as the break-up of the bound state H_t into its constituents

$$H_t \longrightarrow C_t + x \; . \tag{II.55}$$

The radial variable associated with this break-up is

$$\vec{r}_t = \vec{r}_{C_t x} = \vec{r}_{Bx} \text{(pick-up)}$$
$$= \vec{r}_{Ax} \text{ (stripping)} \quad . \tag{II.56}$$

Introduce a complete set of states

$$\Phi^{n_t \ell_t}_{m_t} (\vec{r}_t) = \phi_{n_t \ell_t} (r_t)\, Y^{\ell_t}_{m_t} (\hat{r}_t) \tag{II.57}$$

describing the bound-state wave-function of x and C_t. Here $\phi_{n\ell}$ is the bound-state radial wavefunction defined in Eqs. (II.2 to II.4). Let the transferred nucleons have intrinsic spin J_x and internal quantum numbers x.† The particles emitted (or absorbed) at vertex t are described in terms of the functions

$$\left[\Phi^{n_t \ell_t}(\vec{r}_t) \times \Phi^{xJ_x}(\rho_x) \right]^{J_t}_{M_t} , \tag{II.58}$$

where Φ^{xJ_x} represents the intrinsic structure of x.

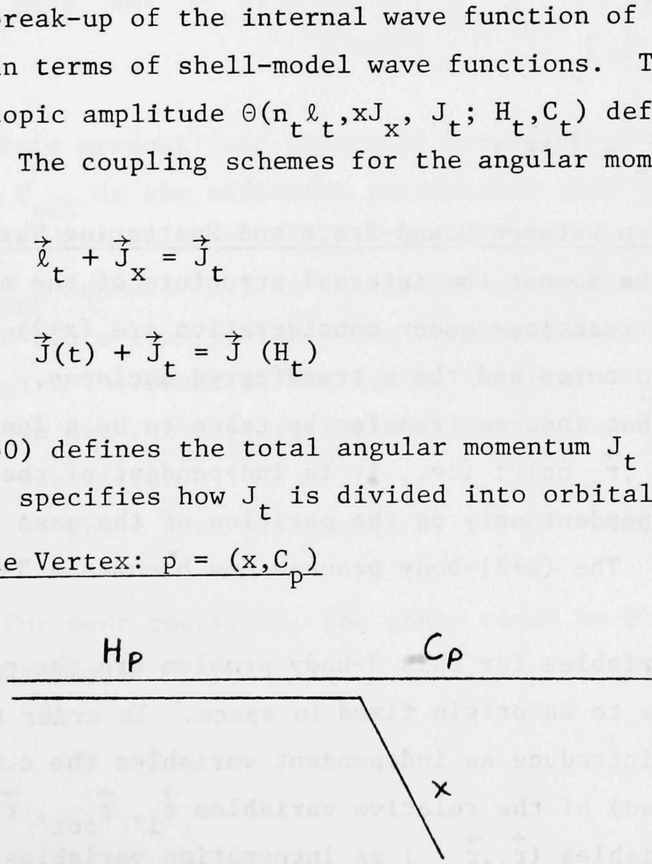
The break-up of the internal wave function of H_t into C_t + x is to be described in terms of shell-model wave functions. This is characterized by a spectroscopic amplitude $\Theta(n_t\ell_t, xJ_x, J_t;\, H_t, C_t)$ defined below[Eqs. (II.96) and (II.97)]. The coupling schemes for the angular momenta at vertex t are

$$\vec{\ell}_t + \vec{J}_x = \vec{J}_t \tag{II.59}$$

$$\vec{J}(t) + \vec{J}_t = \vec{J}\,(H_t) \tag{II.60}$$

Equation (II.50) defines the total angular momentum J_t transferred at vertex t; Eq. (II.57) specifies how J_t is divided into orbital and intrinsic components.

(ii) <u>Projectile Vertex: $p = (x, C_p)$</u>



†Also used for the number of transferred nucleons.

As in the treatment of the target vertex, C_p denotes core, H_p composite (heavier) nucleus.

$$C_p = a \text{ (pick-up)} \qquad H_p = b \text{ (pick-up)}$$
$$= b \text{ (stripping)} \qquad = a \text{ (stripping)}. \tag{II.61}$$

Thus the vertex p describes the break-up of the bound state H_p into its constituents

$$H_p \longrightarrow C_p + x \quad . \tag{II.62}$$

The radial variable is

$$\vec{r}_p = \vec{r}_{C_p x} = \vec{r}_{ax} \text{ (pick-up)}$$
$$= \vec{r}_{bx} \text{ (stripping)} \quad . \tag{II.63}$$

The equations describing the state of the particles emitted (or absorbed) at p are obvious analogs of Eqs. (II.57) and (II.58). The equations analgous to Eqs. (II.59) and (II.60) for the angular momentum $\vec{J}_p$ transferred at vertex p are:

$$\vec{\ell}_p + \vec{J}_x = \vec{J}_p \tag{II.64}$$

$$\vec{J}(C_p) + \vec{J}_p = \vec{J}\,(H_p) \tag{II.65}$$

3. Vector Transformation between Bound-State and Scattering Variables

Ignoring for the moment the internal structure of the nuclear states C_p and C_t, the transfer reactions under consideration are (x+2)-body processes—the "bodies" are the two cores and the x transferred nucleons. Now let the effective interaction that induces transfer be taken to be a function of the bound-state variables $\vec{r}_p,\vec{r}_t$ only; i.e., it is independent of the internal coordinates ρ_x of x, dependent only on the position of the mass center of the x transferred nucleons. The (x+2)-body process now becomes a 3-body process (C_p, C_t and x).

The natural variables for this 3-body problem are the position vectors of C_p, C_t and x relative to an origin fixed in space. In order to separate the center-of-mass motion, introduce as independent variables the c.m. position vector $\vec{R}$ and two (any two) of the relative variables $\vec{r}_i$, $\vec{r}_{out}$, $\vec{r}_t$, $\vec{r}_p$. Ptolemy uses the scattering variables $(\vec{r}_i,\vec{r}_{out})$ as integration variables. The Jacobian of the transformation

$$(\vec{R}_{C_t}, \vec{R}_{C_p}, \vec{R}_x) \to (\vec{R}, \vec{r}_i, \vec{r}_{out}) \tag{II.66}$$

is

$$J = \alpha^3$$

where $$\alpha = \frac{H_p H_t}{(C_p+C_t+x)x} \tag{II.67}$$

and is included in the expression (II.68) for the transformation function H.

With $\vec{r}_i$, $\vec{r}_{out}$ as independent variables, angular-momentum functions of $\vec{r}_p, \vec{r}_t$ must be expressed in terms of $\vec{r}_i$, $\vec{r}_{out}$. This involves evaluation of the coefficients $H^{n_t \ell_t n_p \ell_p}_{L_i L_{out} L_x}(r_i, r_{out})$ of the vector transformation

$$\alpha^3 \phi_{n_t \ell_t}(r_t) V_{eff} \phi_{n_p \ell_p}(r_p) \left[Y^{\ell_t}(\hat{r}_t) \times Y^{\ell_p}(\hat{r}_p)\right]^{Lx}_{Mx}$$

$$= \sum_{L_i L_{out}} (-)^{\frac{1}{2}(L_i+L_{out}+\ell_p-\ell_t)} H^{n_t \ell_t n_p \ell_p}_{L_i L_{out} L_x}(r_i, r_{out}) \left[Y^{L_i}(\hat{r}_i) \times Y^{L_{out}}(\hat{r}_{out})\right]^{Lx}_{Mx} \tag{II.68}$$

of the bound-state product into spherical harmonics of the independent variables $\vec{r}_i, \vec{r}_{out}$. Here V_{eff} is the effective interaction that induces the transition. It will be defined below [Eqs. (II.85) and (II.86)]; all that is of consequence here is that V_{eff} depends only on the radial variables. $H(r_i, r_{out})$ is referred to as the bound-state form factor. The strange phase factor in Eq. (II.68) is introduced to give the phase of the radial integrals I_{L_i, L_{out}, L_x} [Eq. (II.93)] the following two desirable features for large values of L_i and L_{out} [suppressing for the moment the factor $e^{i(\sigma_i+\sigma_{out})}$]:

1) The phase does not change by π every time L_i and L_{out} change by unity.

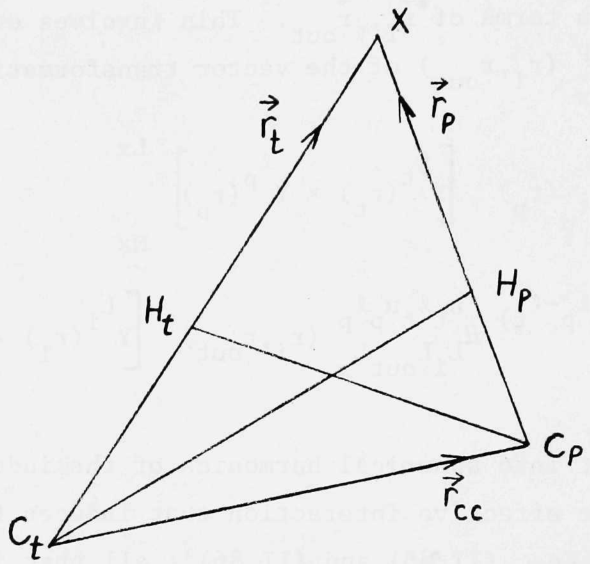
2) For most reactions, the phase tends to 0 from above as both L_i and L_{out} increase.

4. Calculation of Bound-State Form Factor

The procedure for computation of the form factor H in Eq. (II.68) is that of Balian and Brézin.[5] First, $\vec{r}_t$ and $\vec{r}_p$ must be expressed in terms of $\vec{r}_i$ and $\vec{r}_{out}$

$$\begin{pmatrix} \vec{r}_t \\ \vec{r}_p \end{pmatrix} = \begin{bmatrix} s_1 & t_1 \\ s_2 & t_2 \end{bmatrix} \begin{pmatrix} \vec{r}_i \\ \vec{r}_{out} \end{pmatrix} . \tag{II.69}$$

To identify the constants s_i, t_i consider the plane triangle whose vertices are the three basic particles C_t, C_p and x.

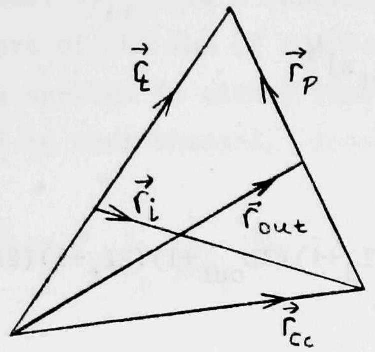


H_t and H_p are at the mass centers of (C_t, x) and (C_p, x). The vectors $\vec{r}_i$ and $\vec{r}_{out}$ have different identifications for pickup and stripping:

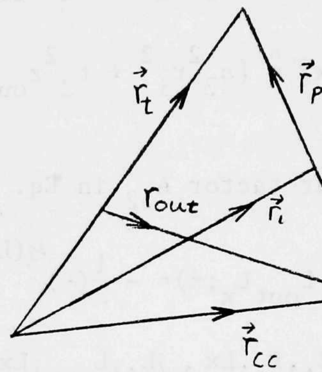
$$\left.\begin{aligned} \vec{r}_i &= \vec{r}_{Aa} = \vec{r}_{H_tC_p} \\ \vec{r}_{out} &= \vec{r}_{Bb} = \vec{r}_{C_tH_p} \end{aligned}\right\} \text{pick-up} , \tag{II.70}$$

$$\left.\begin{aligned} \vec{r}_i &= \vec{r}_{Aa} = \vec{r}_{C_tH_p} \\ \vec{r}_{out} &= \vec{r}_{Bb} = \vec{r}_{H_tC_p} \end{aligned}\right\} \text{stripping} . \tag{II.71}$$

Pick-up



Stripping



Then with α defined by Eq. (II.67) and

$$\gamma = \frac{C_p}{H_p} \qquad \delta = \frac{C_t}{H_t} \tag{II.72}$$

$$\begin{bmatrix} s_1 & t_1 \\ s_2 & t_2 \end{bmatrix} = \alpha \begin{bmatrix} -\gamma & 1 \\ -1 & \delta \end{bmatrix} \quad \text{(pick-up)}$$

$$= \alpha \begin{bmatrix} 1 & -\gamma \\ \delta & -1 \end{bmatrix} \quad \text{(stripping)} \tag{II.73}$$

The bound-state form factor is then given by

$$H^{n_t \ell_t n_p \ell_p}_{L_i L_{out} L_x}(r_i, r_{out}) = \alpha^3 \int_{-1}^{1} dx$$

$$\times A_{12}(\ell_t \ell_p L_i L_{out} L_x ; x) \left\{ \phi_{n_t \ell_t}\left[r_t(x)\right] V_{eff}\, \phi_{n_p \ell_p}\left[r_p(x)\right] \right\} \tag{II.74}$$

where

$$x = \cos\phi = \hat{r}_i \cdot \hat{r}_{out} \tag{II.75}$$

and r_t, r_p are functions of x through

$$r_t(x) = [s_1^2 r_i^2 + t_1^2 r_{out}^2 + 2s_1 t_1 r_i r_{out} x]^{\frac{1}{2}} \quad ,$$

$$r_p(x) = [s_2^2 r_i^2 + t_2^2 r_{out}^2 + 2s_2 t_2 r_i r_{out} x]^{\frac{1}{2}} \quad . \tag{II.76}$$

The angular factor A_{12} in Eq. (II.74) is:

$$A_{12}(\ell_t \ell_p L_i L_{out} L_x; x) = -\frac{1}{2}(-)^{\frac{1}{2}(L_{out}+L_i+\ell_p-\ell_t)} [(2L_i+1)(2L_{out}+1)(2\ell_t+1)(2\ell_p+1)]^{\frac{1}{2}}$$

$$\times \sum_{M_x \mu m} \begin{pmatrix} \ell_t, \ell_p, Lx \\ m, M_x-m, -M_x \end{pmatrix} \begin{pmatrix} L_i, L_{out}, Lx \\ \mu, M_x-\mu, -M_x \end{pmatrix} \Lambda^{\ell_p}_{M_x-m} \Lambda^{\ell_t}_{m} \Lambda^{L_i}_{\mu} \Lambda^{L_{out}}_{M_x-\mu}$$

$$\times \cos\,[m\phi_t + (M_x-m)\phi_p - \mu\phi] \quad , \tag{II.77}$$

where ( ) are 3j-symbols, ϕ is defined by Eq. (II.75), and

$$\phi_t = (-)^S \cos^{-1}(\hat{r}_t \cdot \hat{r}_{out}) = (-)^S \cos^{-1}\left[\frac{s_1 r_i x + t_1 r_{out}}{r_t}\right] \quad ,$$

$$\phi_p = (-)^S \cos^{-1}(\hat{r}_p \cdot \hat{r}_{out}) = (-)^S \cos^{-1}\left[\frac{s_2 r_i x + t_2 r_{out}}{r_p}\right] \quad . \tag{II.78}$$

In the above ϕ and $\cos^{-1}$ are between 0 and π and

$$(-)^S = -1 \quad \text{(pick-up)} \quad ,$$

$$= +1 \quad \text{(stripping)} \quad . \tag{II.79}$$

Finally,

$$\Lambda^k_q = 0 \text{ if } k \pm q \text{ is odd} \quad ,$$

$$= (-)^{\frac{k+q}{2}} \frac{[(k+q)!\ (k-q)!]^{\frac{1}{2}}}{2^k (\frac{k+q}{2})!\ (\frac{k-q}{2})!} \text{ if } k \pm q \text{ is even.} \tag{II.80}$$

5. <u>DWBA Amplitude and Effective Interaction</u>

The transfer amplitude in DWBA has the form

$$T(\vec{k}_i \rightarrow \vec{k}_{out})$$

$$= J \iint d^3r_i d^3r_{out} [\chi^-(k_{out}, r_{out})]^* \langle B,b|V_{eff}|A,a\rangle \chi^+(\vec{k}_i, \vec{r}_i) \tag{II.81}$$

where $\langle V_{eff} \rangle$ denotes a matrix element with respect to all internal core coordinates; $\langle V_{eff} \rangle$ is a function of $\vec{r}_t$ and $\vec{r}_p$. The transition operator V_{eff} is the part of the sum of two-body interactions between constituents of the colliding species in either channel that is not contained in the optical potential in that channel. According to Eqs. (II.70) and (II.71):

$$V_{eff} = \sum_{i \varepsilon C_p} \sum_{j \varepsilon H_t} V_{ij} - U_{opt}(r_{C_p H_t}) \ ,$$

or (II.82)

$$V_{eff} = \sum_{i \varepsilon C_t} \sum_{j \varepsilon H_p} V_{ij} - U_{opt}(r_{C_t H_p}) \ .$$

Two standard approximations are then made.

(i) The additional particles x have little influence on the core-core optical potential. U_{opt} thus describes the core-core interaction.

$$U_{opt} \simeq \sum_{i \varepsilon C_p} \sum_{j \varepsilon C_t} V_{ij} \ , \tag{II.83}$$

and thus

$$V_{eff} \simeq \sum_{i \varepsilon C_p} \sum_{j \varepsilon x} V_{ij} \ ,$$

or (II.84)

$$V_{eff} \simeq \sum_{i \varepsilon C_t} \sum_{j \varepsilon x} V_{ij} \ .$$

(ii) The sum of two-body interaction $\sum_{i \varepsilon C} \sum_{j \varepsilon x} V_{ij}$ is replaced by a one-body potential $V(\vec{r}_{Cx})$ depending only on the relative position of the mass center of x to that of the core

$$V_{eff} \simeq V_{C_p x}(r_p) \ ,$$

or (II.85)

$$V_{eff} \simeq V_{C_t x}(r_t) \ .$$

It is the second approximation that reduces x-nucleon transfer to a three-body problem.

In the simplified form (II.85) V_{eff} can be associated with one or the other vertex. For the one-body potential V_{Cx}, Ptolemy uses the potential that binds the composite system H at the appropriate vertex.

It is known that the approximation (II.83) is poor for the Coulomb part of the interaction. In this case a simple correction[6] can be made;

$$V_{eff} \simeq V_{C_p x}(r_p) + \Delta V \quad ,$$

or

$$V_{eff} \simeq V_{C_t x}(r_t) + \Delta V \quad , \tag{II.86}$$

where

$$\Delta V = V(r_{cc}) - V_{opt}. \tag{II.87}$$

In Eq. (II.87) V_{opt} is the appropriate optical potential as indicated in the following table:

	Pick-up	Stripping
Interaction at p Vertex	$V_{opt}(r_i)$	$V_{opt}(r_{out})$
Interaction at t Vertex	$V_{opt}(r_{out})$	$V_{opt}(r_i)$

$V(r_{cc})$ is the optical potential between the two cores and is evaluated using the same potential parameters as V_{opt}. With the Coulomb correction ΔV, V_{eff} becomes a function of r_p, r_t and x in a fashion which adds no essential complication to the integral in (II.74).

6. Angular Momenta

The angular momenta transferred at the vertices, J_t and J_p have been defined in Eqs. (II.60) and (II.65). The total transferred angular momentum L_x is defined by

$$\vec{L}_x + \vec{J}_p = \vec{J}_t \tag{II.88}$$

The multipole or angular-momentum decomposition of the DWBA amplitude and cross section is based on the total angular-momentum transfer.

7. Differential Cross Section

$$\frac{d\sigma}{d\Omega}(\theta) = \frac{1}{E_i E_{out}} \frac{k_{out}}{k_i} R \sum_{J_t J_p} \sum_{L_x M_x} \left| G_{M_x}^{L_x(J_t J_p)}(\theta) \right|^2 \tag{II.89}$$

where R is a spin-statistical factor:

$$R = \frac{2J_b+1}{2J_a+1} \text{ (pick-up)} \quad ,$$

$$= \frac{2J_B+1}{2J_A+1} \text{ (stripping)} \quad . \tag{II.90}$$

In Ptolemy only one value of J_t and J_p is allowed and the sum over J_t and J_p in (II.89) consists of only one term.

The multipole transition amplitude G is a sum of products of spectroscopic and geometrical components

$$G_{M_x}^{L_x(J_tJ_p)}(\theta)$$

$$= \sum_{n_t\ell_t n_p\ell_p} A_{L_xJ_tJ_p}(n_t\ell_t n_p\ell_p)\, B_{M_x}^{L_x(J_tJ_p)}(n_t\ell_t n_p\ell_p;\theta) \quad . \tag{II.91}$$

summed over all contributing states of orbital motion of the transferred nucleons at each vertex. Ptolemy allows only one projectile and target bound state so the sum in (II.91) consists of only one term. With the phase convention introduced earlier, G is the negative of the amplitude used in Ref. 4.

8. Geometrical Component (including radial integrals)

The angular dependence of the cross section is contained in the "geometrical" component of (II.91):

$$B_{M_x}^{L_x(J_tJ_p)}(n_t\ell_t n_p\ell_p;\theta)$$

$$= \sqrt{4\pi}\; i^{L_x+\ell_t-\ell_p} \sum_{L_iL_{out}} C_{M_x,-M_x,0}^{L_{out},L_x,L_i}\, I_{L_iL_{out}L_x}(n_t\ell_t n_p\ell_p)\, Y_{-M_x}^{L_{out}}(\theta) \quad . \tag{II.92}$$

The radial integrals are expressed in terms of the bound-state form factor H [Eqs. (II.74) to (II.80)] and the radial scattering functions by

$$I_{L_i L_{out} L_x}(n_t \ell_t n_p \ell_p) = e^{i(\sigma_i + \sigma_{out})}$$

$$\times \iint r_i dr_i r_{out} dr_{out} f_{L_i}(r_i) \, H_{L_i L_{out} L_x}^{n_t \ell_t n_p \ell_p}(r_i, r_{out}) \, f_{L_{out}}(r_{out}) \ . \tag{II.93}$$

Note that $B_{M_x}^{L_x}$ is independent of the shell-model wave functions of the nuclear states.

9. Spectroscopic Factors and Spectroscopic Component

Let the states, A, a, B, b be represented by shell-model wave functions. In order to treat the center-of-mass variable $\vec{R}$ consistently and to separate internal and center-of-mass variables of the nuclear states, use harmonic-oscillator shell-model wave functions with the center-of-mass motion in its ground (0s) state.

Consider then the internal states at the target vertex. If J_t is the total A.M. transfer at that vertex, let $\Psi_{M_t}^{\gamma_t J_t}$ be a complete set of x-nucleon shell-model states for the transferred nucleons, and let $a^+(\gamma_t J_t M_t)$ be the creation operators that produce these states from the vacuum. The x-nucleon states must be projected onto states of the transferred nucleons of the form (II.58), with internal and center-of-mass variables separated. Define the necessary coefficients

$$K_{J_t}(n_t \ell_t \ x \ J_x; \gamma_t)$$

$$= \iint d^3R_x d^3\rho_x ([\Phi^{n_t \ell_t}(\vec{R}_x) \times \Phi^{xJ_x}(\rho_x)]_{M_t}^{J_t})^* \ \Psi_{M_t}^{\gamma_t J_t}(\{\vec{r}_\alpha\}) \tag{II.94}$$

where $\{\vec{r}_\alpha\}$ is a set of nucleon coordinates and

$$R_x = \frac{1}{x} \sum_{\alpha=1}^{x} \vec{r}_\alpha \ . \tag{II.95}$$

Then the conventional spectroscopic amplitude $\sqrt{S}$ is given by

$$\sqrt{S}(n_t \ell_t, xJ_x, J_t; H_t, C_t)$$

$$= \sum_{\gamma_t} K_{J_t}(n_t \ell_t x J_x; \gamma_t) \ \langle J(H_t) || A^+(\gamma_t J_t) || J(C_t) \rangle \tag{II.96}$$

(The reduced matrix element is defined by the Wigner-Eckart theorem in the form $\langle jm|T^k_q|j'm'\rangle = C^{j'kj}_{m'qm} \langle j||T^k||j'\rangle$.)

The treatment of the centers of mass leading to Eqs. (II.94) and (II.96) is exact if the shell-model wave functions and the radial functions Φ in Eq. (II.57) and its projectile analog are harmonic-oscillator functions. However, the radial functions of the target and projectile bound states are eigenfunctions of Woods-Saxon potentials. This difficulty is usually ignored since the level of precision of the entire analysis (in particular of its absolute normalization) is seldom high enough to require consideration of such niceties. A crude correction factor can be introduced by expanding the Woods-Saxon wave functions in terms of oscillator functions and assuming that one term dominates. It can then be shown that the replacement

$$\sqrt{S(n_t\ell_t, xJ_x, J_t; H_tC_t)} \rightarrow \Theta(n_t\ell_t, xJ_x, J_t; H_tC_t)$$
$$\Theta(H_tC_t) = \left(\frac{H_t}{C_t}\right)^{\frac{2n_t+\ell_t}{2}} \sqrt{S(H_tC_t)} \quad . \tag{II.97}$$

should correct for the use of the oscillator shell-model wave functions. The projectile vertex is handled in the same way.

In Ptolemy, the spectroscopic amplitudes Θ are read in directly; they can often be inferred from suitable light-ion reactions between the nuclear state in question. Note that S as defined above reduces to the standard spectroscopic factor in the case of single-nucleon transfer.

The spectroscopic component A [Eq. (II.91)] is given in terms of the spectroscopic amplitudes Θ [Eqs. (II.96) and (II.97)] by

$$A_{L_xJ_tJ_p}(n_t\ell_t n_p\ell_p) = \sqrt{2L_x+1} \sum_{xJ_x} (-)^{J_x-J_p+\ell_p+\ell_t}$$
$$\times W(\ell_tJ_t\ell_pJ_p;J_xL_x)\, \Theta(n_t\ell_t, xJ_x, J_t:H_tC_t)\, \Theta\,(n_p\ell_p, xJ_x, J_p:H_pC_p) \tag{II.98}$$

A is independent of the scattering angle and M_x.

10. Outline of Steps in a DWBA Computation for Transfer Reactions.

The main steps in a DWBA transfer reaction calculation can be schematically summarized as follows. In practice a number of these steps are carried out in parallel.

1) Adjust the potentials at the interaction vertices to reproduce the experimental separation energies and compute the bound-state wave functions. This

specifies the effective transition operator through Eqs. (II.85) or (II.86).

2) For given optical-model parameters, solve Eqs. (II.7)-(II.9) for the radial scattering functions. At this stage elastic-scattering amplitudes and cross sections can also be computed.

3) Use Eqs. (II.74) to (II.80) to compute the bound-state form factors $H(r_i, r_{out})$.

4) Fold the bound-state form factors with the radial scattering functions and integrate [Eq. (II.93)] to obtain the radial integrals $I_{L_i L_{out} L_x}$.

5) Using given spectroscopic amplitudes Θ compute the spectroscopic components A_{L_x} of the multipole amplitudes using Eq. (II.98).

6) Calculate the geometrical components $B_{M_x}^{L_x}$ of the multipole amplitudes using Eq. (II.92).

7) Construct the multipole components of the transition amplitude using Eq. (II.91) and compute the cross section [Eq. (II.89)].

Note that in heavy-ion calculations, more than 90% of the time is spent carrying out steps (3) and (4)—construction of the bound-state form factors and integration over r_i and r_{out}.

D - Constants and Units

Ptolemy uses the values:[7]

$$\hbar c = 197.32858 \text{ MeV fm} \tag{II.99}$$

$$M = 931.5016 \text{ MeV}/c^2 \tag{II.100}$$

$$\alpha^{-1} = 137.03604 \tag{II.101}$$

where M is the atomic mass unit and α is the fine-structure constant. Ptolemy reads, stores and prints quantities in the following units:

Quantity	Unit
angles	degrees (input,output)
	degrees or radians (internal)
cross sections	mb
lengths, radii	fm
momenta	fm^{-1}
energies	MeV
reduced mass	MeV/c^2
nuclear masses	amu

potentials	MeV
$B(E,L_x)$	$e^2b^{L_x}$
wave functions:	
bound state (ϕ)	$fm^{-3/2}$
scattering (f, χ)	none
elastic amplitudes (F, B)	fm
amplitudes (G, B)	MeV fm
radial integrals (I)	MeV fm
transfer form factors (H)	MeV fm^{-3}
inelastic effective interaction (H)	MeV

Note that since cross sections are expressed in mb, a factor of 10 is necessary in Eqs. (II.12)-(II.14), (II.23)-(II.26), (II.35), and (II.89) to convert from fm^2.

References for Chapter II

1. M. Abramovitz and I. A. Stegun, Handbook of Mathematical Functions (Dover, New York, 1965).
2. M. G. Mayer and J. H. D. Jensen, Elementary Theory of Nuclear Shell Structure, (Wiley, New York, 1955).
3. A. Z. Schwarzschild, E. H. Auerbach, R. C. Fuller and S. H. Kahana, in Proceedings of the Symposium on Macroscopic Features of Heavy-Ion Collisions, Argonne National Laboratory, Report ANL/PHY-76-2, Vol. II, p. 753 (1976).
4. G. R. Satchler, in Lectures in Theoretical Physics, Vol. VIIIc (Univ. of Colorado press, Boulder, 1966).
   N. Austern, Direct Nuclear Reaction Theories (Interscience, New York, 1970).
5. R. Balian and E. Brézin, Nuovo Cimento 61B, 403 (1969).
6. R. M. deVries, G. R. Satchler and J. G. Cramer, Phys. Rev. Letters 32, 1377 (1974).
7. E. R. Cohen and B. N. Taylor, J. Phys. Chem. Ref. Data 2, 663 (1973).

III - Notation and Syntax

A - Notation

Lower case letters cannot be conveniently used as computer input. Thus some changes must be made to the notation established in the previous section for the description of inelastic excitation and transfer reactions. In general lower case letters will simply be converted to upper case. However, in Sec. II a distinction was made between lower- and upper-case letters in the identification of the reaction participants. For Ptolemy input this distinction will be maintained by specifying the target particles as BIGA and BIGB while the projectile particles will be A and B. Thus the reaction computed by Ptolemy may be written as

BIGA(A, B)BIGB .

In the incoming state, the target is referred to as "BIGA" and the projectile is "A". In the final state the residual target is "BIGB" and the ejectile is "B". The exchanged particle is referred to as "X". For a stripping reaction we have

A = B + X,
BIGB = BIGA + X,

while for a pickup reaction

B = A + X,
BIGA = BIGB + X.

Ptolemy will compute either pickup or stripping reactions; it is not necessary for the user to interchange particles to force the reaction into one form or the other. Inelastic excitation is implied if the mass and charge of A and B, and of BIGA and BIGB, are the same.

The projectile or ejectile bound state (whichever is appropriate) is always referred to as the projectile bound state while the target or residual nucleus bound state is called the target bound state. The Q value of the reaction is the difference of the outgoing and incoming kinetic energies in the center of mass system so that in terms of the bound state energies

Q = E(projectile) - E(target) : stripping,
Q = E(target) - E(projectile) : pickup.

Note that Ptolemy deals with actual bound state energies (i.e., negative numbers). In the case of inelastic excitation, the Q-value is, of course, just the negative of the excitation energy.

B - Ptolemy Syntax

Ptolemy uses a free-form keyword-based input. Options are specified and stages of the calculation selected by the specification of the appropriate keyword. Numeric values are entered by the specification of a number entering keyword followed by the desired value. One or more keywords and associated numbers may be included on a single input line+ or a data value may be on the line following its keyword. (The CHANNEL, REACTION and HEADER keywords are exceptions and require associated information to be on the same input line.) Words and numbers may not be split across two lines and they may not contain imbedded blanks. In both TSO and batch usage, Ptolemy uses only the first 72 positions of the input line; the last 8 are reserved for optional line numbers that will be printed but otherwise ignored.

Keywords may be separated from other keywords on the same line by blanks, commas, or sequences of blanks and commas. The equal sign may be used (but is not required) between a keyword and its associated data value. The colon may be used following the CHANNEL, REACTION and HEADER keywords but should not otherwise be used in Ptolemy input. The semicolon is used to begin a stage of the calculation; it indicates that all input needed for that stage has been provided.

Numerical data may be entered with or without a decimal point and may have the E form of exponent. Valid numerical inputs are

2, 2.3, .0002, 2E-4, 2.325E+7, -5.3, +7E-5 .

An "E" appearing in a number indicates the beginning of the power of 10 bywhich the number is to be multiplied. Thus

5.3E-7 = 5.3×10^{-7}
1E20 = 10^{+20}

Angular momenta that have the possibility of being half-integer (J or S values but not L values) have a special form of input. They may be either simple integers or integers followed by "/2" to indicate half integer values. They should not be coded with a decimal point. Thus

J = 2, S = 3/2, JP = 4/2

are all valid (the last is the same as JP = 2) while

J = 2., S = 1.5

+ Input lines are either cards in an input deck for a batch run or lines typed at a terminal in TSO usage of Ptolemy.

are both invalid. Such J and S values may be followed by a parity sign which will be ignored. Thus

J = 2, J = 2-, and J = 2+

are all equivalent.

Keywords may have more than eight characters in their names but only the first 8 characters are used and required. Keywords never have embedded blanks in their names.

Comments may be placed anywhere in the input. They are preceded by a dollar sign ($) which indicates that the rest of the input line is a comment. If a second dollar sign appears on the same line, the comment is terminated and the remainder of the line is processed as normal input.

IV - Elastic and Bound State Calculations

The basic ingredients of the DWBA calculations performed by Ptolemy are two-body wavefunctions -- optical-model scattering states for inelastic excitation and both bound-state and optical-model scattering states for transfer. Obviously, optical-model scattering states are also used in the optical model fitter.

One may use the facilities of Ptolemy to compute the properties of two-body bound or scattering states without doing a larger scale calculation. Such calculations will be referred to as "stand-alone" two-body calculations. Wherever possible the same keywords and conventions are used for defining the two-body states that are components of a larger calculation as are used in stand-alone two-body calculations. Examples are the definitions of the potentials and the specification of the integration grid used to solve the Schroedinger equation. For this reason we describe the stand-alone two-body calculations before progressing to the more complicated calculations -- the material introduced in this chapter will be refered to in many of the succeeding chapters.

A - Specifying the Two-Body Channel

Stand-alone two-body calculations are done by defining the two particles and the potential that acts between them and then entering a semicolon to start the calculation. If the energy is negative a bound state calculation will be made, if it is positive the two-body scattering will be computed. If desired one may use the keywords BOUNDSTATE or SCATTERING to indicate which is to be done and the energy will be checked for validity. Although it is possible to mix stand-alone and DWBA calculations in one job, it is recommended that separate jobs be used for stand-alone and complete DWBA runs. However many stand-alone calculations of both bound states and scattering may be done in one job.

The two particles involved in the stand-alone calculation are referred to as the "projectile" and "target." These words have their customary meanings for scattering states; the only distinction for bound states is that the projectile's angular momentum is used to determine the spin-orbit force.

The CHANNEL keyword may be used to specify the nuclei in the two-body state. Some examples will illustrate its form:

```
CHANNEL  12C + 208PB
CHANNEL:  P + 11B = C12
CHANNEL = 209BI(7/2- .9) = P + 208PB
```

The first example gives a scattering state while the other two define bound states. Note that in the case of bound state channels, the resultant bound state may be either the first nucleus (inwhich case it is followed by an equal sign) or the last nucleus. In all cases the projectile and target must be separated by a plus sign and <u>the projectile always comes first</u>. If a bound state is being specified, the composite nucleus may be either first or last and must be separated from the other two nuclei by an equal sign.

The nucleides are defined by an element symbol consisting of the atomic weight and a one- or two-character element abbreviation. The atomic weight may either precede or follow the symbol but no blank spaces or other punctuation may intervene. In addition the following symbols (without atomic weights) may be used:

N - neutron,
P - proton,
D - deuteron,
T - triton,
H - ^{3}He,
A - ^{4}He.

Excited states may be indicated by enclosing the spin and excitation energy in parentheses following the element symbol. The left parenthesis for excited state specification must immediately follow the element symbol. The excitation energy and spin of the excited state may be given in either order, and the excitation energy must include a decimal point even if it happens to be an integer. Excitation energies are given in MeV. Any or all of the two or three nuclei may be given an excited state specification. The CHANNEL keyword and the complete channel specification must be contained on a single input line.

The CHANNEL keyword will define the projectile, target and bound-state mass, charge, and intrinsic spin. The intrinsic spins and the ground-state mass excesses of the nucleii are found from the 1975 Oak Ridge Atomic Mass Adjustment and the 1971 Nuclear Wallet Cards compilation+. In addition for bound states the total angular momentum and the bound-state (cluster separation) energy are also defined.

If the CHANNEL keyword is not used, the particle masses may be entered with the keywords MP and MT which give the masses in AMU of the projectile and target respectively. The masses do not need to be integers. Alternatively one can use the keyword "M" to enter the reduced mass in MeV/c². The charges of the two particles may be entered with the keywords ZP and ZT. The excitation energies may be entered using the keywords E*P and E*T; if they are not

---

+ F. Serduke, "Atomic Mass Table," Argonne Internal Report, 1975, and private communication.

entered, zero will be used. The projectile and target intrinsic spins may be entered with the keywords SP and ST. The total angular momentum of a bound state may be entered with the keyword "J." It is not necessary to enter J or ST (the calculation does not depend on them) and SP is necessary only if there is a spin-orbit force.

The projectile and target will be recognized as identical if they have the same mass, charge, spin, and excitation energy. In such cases the appropriate spin statistics will be used for scattering calculations. Non-identical particle scattering may be forced by specifying a small excitation energy for one of the particles.

The c.m. energy may be entered by using either of the keywords ECM or E. In the case of bound states one of these should be used to enter the energy as a negative number unless the CHANNEL keyword is used. The laboratory scattering energy may be entered with the keyword ELAB. In this case both MP and MT must be defined to allow the conversion to the c.m. energy.

The number of nodes and orbital angular momenta of bound states must be defined for bound state calculations. The keyword NODES is used to specify the number of nodes. The node at the origin is not included in the count so that the lowest bound state for each value of L has 0 nodes. The keyword "L" is used to specify the orbital angular momentum of the bound state. If a spin-orbit force is being used in the bound state, it is necessary to enter the total angular momentum of the "projectile". This is done with the keyword JP. Jp, L and Sp are used to find the value of L•S in the spin-orbit force. If either of St (the target spin) or J (the total bound state spin) are zero, then Jp need not be specified since it will be uniquely determined by other known spins.

B - Specifying the Potentials

The potentials are defined by the keywords Vi, Ri or Ri0, and Ai where the suffix "i" indicates the potential that is being defined. Possibilities for "i" are:

1) (null) - no suffix refers to the real part of the Woods-Saxon well.
2) I - The suffix I refers to the imaginary part of the Woods-Saxon well.
3) SO - The suffix SO designates the real part of the spin-orbit force.
4) SOI - Imaginary part of the spin-orbit force.
5) SI - Imaginary surface potential.
6) C - Coulomb potential (VC and AC are not defined).

The forms of these potentials are as follows:

1) Real part of the Woods-Saxon:
```
- V / (1 + X)
X = exp[ (r-R)/A ]
```

2) Imaginary part of the Woods-Saxon (volume absorption):
```
- VI / (1 + XI)
XI = exp[ (r-RI)/AI ]
```

3) Real part of the spin-orbit:
```
+ (VSO+TAU*V) * 4L•S * (1/r) * (d/dr) 1/(1+XSO)
XSO = exp[ (r-RSO)/ASO ]
```

4) Imaginary part of the spin-orbit:
```
+ (VSOI+TAUI*VI) * 4L•S * (1/r) * (d/dr) 1/(1+XSOI)
XSOI = exp[ (r-RSOI)/ASOI ]
```

5) Imaginary surface potential (surface absorption):
```
+ VSI * 4*ASI * (d/dr) 1/(1+XSI)
XSI = exp[ (r-RSI)/ASI ]
```

6) Coulomb potential

a) point and uniform sphere:
```
+ Zp*Zt * e² / r                              : r ≥ RC
+ Zp*Zt * e² * {3 - (r/RC)²} / (2RC)          : r < RC
```

b) two uniform spheres:
```
+ Zp*Zt * e² * 9 / (16 pi² RCP³ RCT³ )
  * Integral(0, RCP) d³rp  Integral(0, RCT) d³rt
    1 / |r-rp-rt|
```

where

L•S = (Jp(Jp+1) - L(L+1) - Sp(Sp+1)) / 2 .

The potential well depths are given in MeV. Note that the spin-orbit well depths may either be specified directly by using the VSO and VSOI keywords or their ratio to the corresponding Woods-Saxon depths may be given by using the TAU and TAUI keywords. The TAU's are related to the LAMBDA's of DWUCK and LOLA by

TAU = LAMBDA/(4*45.2)

Note that VSO and VSOI have dimensions of MeV since the factor "4" in the definition of the spin-orbit force is interpreted as 2*2 where one "2" converts L•S to L•sigma, and the other "2" is approximately the square of the pion Compton wavelength in fm. The ratio TAU is dimensionless. The spin-orbit force always refers to the spin of the projectile coupled to its orbital angular momentum; the spin of the target does not enter the potential. A spin-orbit force may not be used if the particles are identical.

In all cases the radius parameter (R0, RI0, RSO0, RSOI0, RSI0, RC0, RCOP, or RCOT) may be entered in place of the potential radius. The radius is then computed as

$$R = R0 * Mt^{**}(1/3) \quad : Mp \le 2 ,$$
$$R = R0 * \{ Mp^{**}(1/3) + Mt^{**}(1/3) \} \quad : Mp \ge 3 .$$

These formulas are generally appropriate for optical potentials, but may result in unexpectedly large potential radii for bound states of a nucleon cluster (such as an alpha particle) and a heavier core.

Defining RC or RC0 causes the "point and uniform sphere" Coulomb potential (6a) to be used; otherwise the "two uniform spheres" (6b) potential is used. In the latter case, the radius of each nucleus may be explicitly entered with the RCP and RCT or RCOP and RCOT keywords, or they may be left undefined. If they are not defined, Ptolemy will choose them to give RMS radii roughly consistent with those determined by electron scattering. These radii are taken to be:

$1 \le A \le 2$	R = 0 ;
$3 \le A \le 16$	Values from Landolt-Boernstein+ ;
$17 \le A$	Values from Bohr and Mottelson formula++ .

The Coulomb potential between two uniform spheres is not available for bound states.

The real and imaginary potential parameters may be given a dependance on the laboratory energy by the use of keywords that end in "E" or "ESQ." In this case the quantities to be used in the above equations will be computed as follows:

$$\begin{aligned}
A &= A + AE*Elab + AESQ*Elab^2 ,\\
R0 &= R0 + R0E*Elab + R0ESQ*Elab^2 ,\\
V &= V + VE*Elab + VESQ*Elab^2 ,\\
AI &= AI + AIE*Elab + AIESQ*Elab^2 ,\\
RI0 &= RI0 + RI0E*Elab + RI0ESQ*Elab^2 ,\\
VI &= VI + VIE*Elab + VIESQ*Elab^2 .
\end{aligned}$$

The names appearing on the right of the equal signs in the above equations are the keyword values the user enters. The quantities on the left are then used to evaluate the potentials. The default value for all the keywords ending in "E" or "ESQ" is 0.

+ R. Hofstadter and H. R. Collard in Landolt-Boernstein, Numerical Data and Functional Relationships in Science and Technology, Vol. 2, K.-H. Hellwege, ed. (Springer Verlag, 1967). Average values of the entries in column 5 of Table 2.1, pp 32 - 34, are used.

++ A. Bohr and B. Mottelson, Nuclear Structure, Vol. I, (Benjamin, New York, 1969), pp 160 - 161.

| The keyword EINVERSES may be used to indicate that 1/Elab and
| 1/Elab^2 are to be used in the above formulas for the energy
| dependent parameters. The default is EPOWERS which results in the
| above formulas.

If Ai and/or both Ri and Ri0 are not defined for the imaginary part of a potential, Ptolemy will use the Ai or Ri for the real part of the same potential (RSO will be used for RSOI, A for AI, etc.). If ASO or both RSO and RSO0 are not defined, A or R will be used for them. If ASI or both RSI and RSI0 are not defined, AI or RI will be used for them.

In process of computing the bound state wavefunctions it is necessary that V (the potential depth) and E (the bound state energy) be made consistent with each other. Ptolemy varies one or the other of these two quantities until they are consistent. The keywords FITV and FITE may be used to determine which quantity is to be varied. FITV causes V to be changed to produce a well that has the bound state energy E. If a spin-orbit force has been specified via the keyword TAU, the depth of the spin-orbit force is also varied since the ratio of the spin-orbit force to the Woods-Saxon well is held constant at TAU. On the other hand, if VSO is used to specify the spin-orbit force, the strength of the spin-orbit force is not changed as V is changed. FITE causes E to be computed as the bound state energy of the given potential. The default is FITV.

C - Controling the Calculation

If a scattering calculation is being made, the S-matrix elements will be found for a range of orbital angular momentum values. This range may be explicitly specified by the LMIN and LMAX keywords. If LMIN and/or LMAX are not specified, they will be based on Lcritical (the angular momentum for which |S| = 1/2) which is estimated via semi-classical expressions. In such cases the four keywords LMINMULT, LMINSUB, LMAXMULT, and LMAXADD are used to compute LMIN and/or LMAX from the formulas:

```
LMIN = Min( LMINMULT*Lcritical , Lcritical-LMINSUB ) ,
LMAX = Max( LMAXMULT*Lcritical , Lcritical+LMAXADD ) .
```

Note that if only one of LMIN or LMAX is explicitly specified, then only the other is computed from the above formulas. One should note that the extrapolation to large L-values that is provided in DWBA calculations does not occur in elastic scattering calculations. Thus a larger LMAX or LMAXADD is required for elastic scattering calculations.

It may be desired to compute the elastic S-matrix elements for only one value of L. In such cases, the keyword L should be used to specify the desired value. If a spin-orbit force is entered for a scattering problem, the S-matrices will be computed for all values of Jp connected with each value of L (note that Sp is not limited to 1/2 for spin-orbit forces). If it is desired to have only one value of Jp, the keyword JP may be used to specify that value. If both of the keywords "L" and "JP" are used, only one scattering partial wave will be computed. Bound states are always computed for only one value of L and Jp.

The keyword ELASTIC may be used to cause the elastic differential cross sections to be computed. The default is NOELASTIC which suppresses the differential cross sections. The cross sections are given in millibarns/steradian and as ratios to the corresponding Rutherford (Mott if the particles are identical) cross sections. The cross sections are averaged over the initial spins and summed over the final spins.

The grid of c.m. angles on which the differential cross sections are displayed is controlled by the keywords ANGLEMIN, ANGLEMAX, and ANGLESTEP. The angles are given in degrees. The default values are

```
ANGLEMIN  =  0 ,
ANGLEMAX  = 90 ,
ANGLESTEP =  1 .
```

| The keyword LABANGLES may be used to indicate that ANGLEMIN, ANGLEMAX, and ANGLESTEP specify a grid of laboratory angles. In such cases there is a two to one mapping of laboratory angles to c.m. angles if the projectile mass is greater than the target mass. Ptolemy will convert positive laboratory angles to the smaller c.m. angle and negative angles to the larger c.m. angle. In such cases ANGLEMAX may be negative to cause the c.m. angles to steadily increase through 90°. The default is CMANGLES.

The computation of the two-body wavefunctions (both bound and scattering states) may be controlled with the ASYMPTOPIA and STEPSIZE or STEPSPER keywords. ASYMPTOPIA specifies (in fm) the radius at which the wavefunctions are to be assumed to be asymptotic. It is also the largest value of r for which the wavefunctions will be computed and stored.

The keyword STEPSIZE gives the increment used in the solution of the bound- and scattering-state Schroedinger equations. Since arrays must be constructed that have ASYMPTOPIA/STEPSIZE elements, one should avoid making this ratio very large. The keyword STEPSPER may be used to specify the number of steps to use per wavelength. If it is entered, STEPSIZE will be computed according to the formulas:

```
STEPSIZE = Min( 1/kappa, A ) / STEPSPER  : Bound states
STEPSIZE = Min( lambda, 2*A ) / STEPSPER : Scattering
```

where "kappa" is the bound state inverse range:

kappa = sqrt(2*M*|E|) ,

and "lambda" is the scattering wavelength:

lambda = 2*Pi / sqrt(2*M*E) .

In both cases "A" is the diffuseness of the real part of the central Woods-Saxon well. It is suggested that STEPSPER be used instead of STEPSIZE since then the step size will automatically be adjusted as the wavelength changes due to changes in the scattering energy. If both STEPSIZE and STEPSPER are defined, STEPSPER has precedence.

The keyword PARAMETERSET may be used to select a standard set of values for the calculation-controlling keywords. The keyword is followed by the name of the desired set; Table I gives the names of

TABLE I

PARAMETERSET names and associated values for elastic scattering calculations. The first column gives the default values.

Keyword	Default	EL1	EL2	EL3
LMINSUB	20	15	20	25
LMINMULT	.6	.7	.6	.5
LMAXADD	30	15	20	25
LMAXMULT	1.6	1.6	1.8	2.
ASYMPTOPIA	20	15	20	25
STEPSPER	none	12	15	20
FITACCURACY	10^{-3}	$2*10^{-3}$	$2*10^{-4}$	$2*10^{-5}$

the sets for elastic scattering and the associated values. Individual settings may then be overridden by subsequently entering the appropriate keywords. Note that STEPSPER and not STEPSIZE is defined by these PARAMETERSET sets. Since STEPSPER has precedence over STEPSIZE, one must use the command

UNDEFINE STEPSPER, STEPSIZE = ssss

if one wants to enter a specific STEPSIZE after having used PARAMETERSET (UNDEFINE is defined on page 77). The FITACCURACY keyword in Table I will be explained in the chapter on optical model fits.

D - The Two-Body Wavefunctions

The computed wave functions (for both bound and scattering states) will be printed if the keyword WRITESTEP is used. This keyword specifies the stepsize for which the wavefunction is to be tabulated. The value of WRITESTEP should be a multiple of STEPSIZE (page 39); if it is not, the closest multiple of STEPSIZE will be used. Setting WRITESTEP equal to 0 (the default) will suppress the printing of the wavefunction.

The bound state wavefunctions are the solutions of the Schroedinger equation

```
{ hbar²/(2Mr²) [ -(d/dr)r²(d/dr) + L(L+1) ]
  + V(r) - E } Phi(r) = 0 ,
```

while the scattering wavefunctions are the solutions of

```
{ hbar²/(2M) [ -d²/dr² + L(L+1)/r² ]
  + V(r) - E } f(L)(r) = 0 .
```

The bound state wavefunctions are normalized to unity so that

```
Integral(0 to infinity) dr r² Phi² = 1 .
```

The scattering wavefunctions are normalized to have the asymptotic form

```
| f(r) ---> (1/2) * { (1+S)*F(kr) + i (1-S)*G(kr) } ,
|      =  cos(D) exp(iD) { F(kr) + tan(D) G(kr) } ,
```

| where F and G are the regular and irregular Coulomb functions, and
| D is the complex phase shift [S = exp(2iD)]. If the optical poten-
| tial is real, then the phase shift D is real and the phase of the
| wavefunction is exp(iD) for all r. In this case one might want
| to use the REALWAVE keyword to cause the wavefunctions to be multi-
| plied by exp(-iD) so that

```
f(r) ---> cos(D) F(kr) + sin(D) G(kr)      [REALWAVE]
```

| The default is COMPLEXWAVE. Note that asymptotically the bound state wave functions behave as exp(-kappa*r)/r while the scattering wavefunctions do not have a 1/r in their asymptotic form.

The name of the bound state wavefunction will be PHIn where "n" is an integer that is 1 for the first bound state and is increased by 1 for each subsequent bound state. After n = 9, it is set back to 1 again. Thus one can have up to nine bound state wavefunctions in the allocator at once. The names of the real and imaginary scattering wave functions will be WAVER and WAVEI. If it is desired to have more than one scattering wavefunction in the allocator at once, the keywords RENAME or COPY should be used (see Sec. VIII).

The keyword CHECKASYMPT may be used to cause the rate of convergence of the scattering wavefunctions to the asymptotic form given above to be displayed when the wavefunction is computed. The difference of the exact wavefunction and the asymptotic form will be printed at intervals determined by WRITESTEP (which must also be defined). The keyword NOCHECKASYM cancels a previously entered CHECKASYMPT and is the default.

E - Reading the Output

Ptolemy produces a summary of the two-body channel that for the most part is self-explanatory. The summary contains properties of the nuclei (spin, mass, etc.) and the two-body scattering or bound-state energy. Following this is the potential summary in which there is a line for each non-zero potential. The well depths are given in a column labeled "Coupling Cons."; the entry in this column for the Coulomb potential is the Sommerfeld parameter. If the calculation is of a bound state, the summary is produced after the calculation is complete and thus contains the real well depth (or binding energy if FITE was specified) that is the result of the search for an eigenvalue of the Schroedinger equation.

During the computation of elastic wavefunctions, the S-matrix elements, their magnitudes and phases (in degrees), and the transmission coefficients are tabulated. If the keyword ELASTIC is specified, the tabulation of S-matrix elements is followed by a tabulation of elastic cross sections. In this tabulation scattering angles (in degrees) and differential cross sections are given in both the c.m. and laboratory frames. In addition the c.m. Rutherford cross section and the ratio of the elastic cross section to the Rutherford value are given. If the scattering is of identical particles, then all of the cross sections are suitably symmetrized (the resulting symmetrized Rutherford cross sections are sometimes referred to as Mott cross sections).

The last two columns of this tabulation are labeled "% PER LOW L" and "% PER HIGH L" and contain indications of the errors in the differential cross sections due to the low and high orbital angular momentum limits. They are defined as

```
[% PER LOW L]  = 100*{sigma(LMIN)-sigma(LMIN+2)}/2 ,
[% PER HIGH L] = 100*{sigma(LMAX)-sigma(LMAX-2)}/2 ,
```

and thus are the percent error for omitting the smallest and largest L-value used in the calculation. Experience has shown that the actual error in the cross sections is typically five times the number printed, but such an estimate is strongly dependent on the rate at which |S| is approaching 0 or 1. (Of course, if LMIN=0 the low L error may be ignored.)

Following the differential cross section tabulation, the total reaction cross section and the nuclear total cross section are printed. These quantities are defined in Chapter II.

V - Optical Model Potential Fits

Ptolemy provides a powerful and efficient program for fitting optical model potentials to elastic scattering data. Data for more than one elastic scattering reaction or at more than one bombarding energy may be used in a fit. The optical potentials may be given an energy dependance. The normalization of the data and the laboratory angle calibration may be used as fit parameters.

A - Specifying the Fit Parameters and Data

The input for an optical model fit consists of the following items:

1) specification of the potential parameters that are to be varied in the fit,
2) initial values of the search parameters and the fixed values of all other potential parameters,
3) experimental data,
4) parameters to control the fit and elastic scattering calculations.

Items 1 to 4 may be given in any order. The end of the input for a fit is signaled by a semicolon (;) which causes the fit to begin. When the fit is complete, the potential parameters will be set to the best potential parameters that were found. In addition the predicted optical model scattering cross sections will be printed for each experimental point that was included in the fit. The user may then enter control lines to compute the elastic scattering on a uniform angular grid, or he may increase the accuracy of the calculation (through the use of keywords such as LMINMULT, LMAXADD, STEPSPER or FITACCURACY) and resume the search by entering a second semicolon.

Both the fixed and initial potential parameters are entered using the potential keywords of Section IV-B. The LMINSUB, LMIN, LMAX, LMINMULT, LMAXADD, LMAXMULT, STEPSIZE, STEPSPER and ASYMPTOPIA keywords (Section IV-C) may be used to control the accuracy of the elastic scattering calculations during the search. | Alternatively one of the elastic PARAMETERSET keywords (page 40) | may be used.

The parameters to be varied in the fit are specified by the FIT keyword. This keyword is followed by a list of potential | parameters (page 35) and/or renormalization factors and laboratory | angle shifts to be varied. The list must be enclosed in parentheses. If two or more potential parameters are to be held equal to each other during the fit, they should be joined by an equal sign in the FIT list. Some examples of valid FIT specifications are:

FIT (V VI) - a two-parameter fit;
FIT (A=AI, AE=AIE, V) - a three-parameter fit with the same energy dependance in A and AI;
FIT (R0=RI0=RC0) - a one-parameter fit.

Each FIT parameter must have its initial value explicitly entered by means of the potential-defining keywords of Sec. IV-B. The initial value of the first of a string of equal parameters is the one that will be used to start the search.

The normalization of the data and/or the zero point of the laboratory angles may be treated as fit parameters. If only one group of data is being fitted, the keywords RENORMALIZATION and ANGLESHIFT may be included in the list of FIT parameters to cause these quantities to be included in the search. (See the description of the DATA keyword below for a precise definition of the meaning of ANGLESHIFT.) If there is more than one group of data to be fitted, the keywords RENORMn and/or SHIFTn, where "n" is an integer from 1 to 20, may be used to indicate which group of data is to be adjusted in magnitude and/or angle. If several groups of data are to be adjusted, then there will be several RENORMn's or SHIFTn's in the FIT list; these may be connected with equal signs if the same adjustment is to be made to all of them. The initial values of the renormalizations and shifts that are part of the seach are specified in the DATA keyword (see below). Some examples of fits that include searches on the renormalization or angles are:

FIT (V VI A RENORM) - assumes only one data group.
FIT (R0 RI0 SHIFT1=SHIFT2 RENORM1 RENORM2) - two data groups, both have the same unknown error in angles but possibly different errors in their normalizations.

The default minimizing program (see page 49) cannot be used if the laboratory angle shift is one of the fit parameters. In such cases the POWELL65 or ROCORD minimizer must be specified.

The experimental data are entered using the DATA keyword. This keyword is followed by a pair of parentheses that enclose all of the data that are to be used. As many cards as are necessary may be used to enter the data; the end of the DATA keyword is signalled by the closing paranthesis. If a second DATA keyword occurs in a given job, it will replace, not supplement, the data entered with the first keyword. The data are entered in one or more groups, each containing data for a single elastic channel at a single laboratory energy. Each group is preceded by a list of keywords that give the elastic channel, the laboratory energy, optional overall weight and renormalization factors, and the type of data to be entered. The data then follow these keywords. The start of the next group is indicated by the occurence of a keyword.

The elastic channel is specified by the CHANNEL keyword which is followed by an elastic channel specification (see page 33). The laboratory energy of the group of data is specified using the ELAB keyword and is in MeV. If there is only one group of data, the channel and/or laboratory energy may be specified outside (either before or after) the DATA keyword. Each data item is weighted in the chi-squared sum by the square of the inverse of its experimental error. An overall weight factor that will multiply each of these individual weights may be entered using the WEIGHT keyword. The keyword RENORMALIZATION may be used to enter a renormalization factor that is multiplied into each experimental value before computing the chi-squared sum. If WEIGHT or RENORMALIZATION are not entered, the default value of unity is used.

The laboratory angles of the data can be shifted by a constant angle with the ANGLESHIFT keyword. This keyword specifies an increment (in degrees) that is to be added to each angle in the laboratory frame. [In the Almagest (ca. 130 AD) Ptolemy "updated" the positions of some 1000 stars by shifting the positions of every star by the same amount+.] Input c.m. angles and data are transformed to the laboratory frame for this shift. After the shift, the Jacobian relating the c.m. and laboratory frames is recomputed at the new angle, and the angles and data are transformed back to the c.m. frame. Furthermore if the cross sections are given as ratios to the Rutherford cross sections, the data values are changed to correspond to the Rutherford cross sections at the new angles. Thus this keyword treats the data as if the absolute normalization of the data is experimentally known. If the data was normalized to the Rutherford cross section for small angles, it will be necessary to use the RENORMALIZATION keyword to specify a suitable renormalization factor [the average (over the small angles) of the ratios of the Rutherford cross sections at the original and shifted angles] for the shifted data.

A set of three or four keywords is used to specify the type and order of data being entered. The set must consist of one keyword from each of the following three groups:

1) ANGLE, CMANGLE, LABANGLE;
2) SIGMA, CMSIGMA, LABSIGMA, SIGMATORUTH;
3) ERROR, PERCENTERROR, MBERROR.

In addition a fourth keyword, POLARIZATION, may be used to enter polarization data, but such data will be ignored in the fit. The subsequent data is entered in triples or quadruples of numbers whose order is the same as that of the three or four keywords. These keywords remain in effect until a new set is specified; if any one of them is entered, then a complete new set must be given.

+ R. R. Newton, "The Crime of Claudius Ptolemy," (John Hopkins University Press, 1977).

One of the ANGLE, CMANGLE, or LABANGLE keywords is used to indicate the scattering angles of the data. The ANGLE or CMANGLE keywords are used to designate center-of-mass angles in degrees. The LABANGLE keyword means that laboratory angles in degrees will be given. In this case there are two c.m. angles associated with each laboratory angle if the projectile mass exceeds the target mass. For such cases, positive angles are converted to the smaller possible c.m. angle, while negative angles are converted to the larger. It is not possible to have the cross sections for both c.m. angles added together for comparison with the data.

The type of data that is being entered is indicated by the SIGMA, CMSIGMA, LABSIGMA, or SIGMATORUTH keywords. The first three keywords indicate that cross sections in millibarns are being entered. If SIGMA is used, the cross sections are in the rest frame (c.m. or laboratory) indicated by the ANGLE, CMANGLE, or LABANGLE keywords. The keywords CMSIGMA or LABSIGMA may be used to explicitly indicate the choice of frame or to specify c.m. cross sections at laboratory angles (or vice versa). Ratios of cross sections to the Rutherford (Mott for identical particle scattering) cross sections are indicated by the keyword SIGMATORUTH.

The keywords ERROR, MBERROR or PERCENTERROR are used to indicate the nature of the experimental errors. The ERROR keyword means that errors are being entered in the same units as the data. Thus the errors will be expressed either in millibarns (in the c.m. or laboratory frames as determined by the data) or as a ratio to the Rutherford cross section. The keyword MBERROR indicates that no matter what the data type, the errors are in millibarns. If the data are ratios to Rutherford, then such errors are expressed in the c.m. frame; otherwise the frame is the same as that used for the data. The keyword PERCENTERROR indicates that the errors are expressed in percent.

The following example illustrates the DATA keyword:

```
DATA ( CHANNEL 16O+40CA  ELAB=48
ANGLE PERCENTERROR SIGMATORUTH
  10 5 1.023,  12.5 2 .99  20 3.3 .5
  30  15  .12
  ELAB = 56  WEIGHT = .5   ANGLE SIGMA MBERROR
  10  3.  .3,   15 1. .1  20 .1 .1   )
```

Here we are entering data at two different energies. Both sets of data are for $^{16}O+^{48}Ca$ elastic scattering. The data at the first energy is given at angles of 10, 12.5, 20, and 30 degrees and consists of ratios to the Rutherford cross section that are respectively 1.023, .99, .5, and .12. The errors in these numbers are given as percentages. The data for the second energy are given in millibarns with errors also specified in millibarns. If data that consists of the same quantities in the same order is to be entered at several energies, it is not necessary to repeat the angle, cross section and error keywords for each data group.

B - Controlling the Fit

One of the keywords LMCHOL, QUAVER, MINIM, DAVIDON, POWELL65, or ROCORD may be used to pick the minimizing program that is to make the search. The average user will have need of only the default which is LMCHOL. The keywords FITMODE, FITMULTIPLE, FITRATIO, NUMRANDOM, and REINITIALIZE are used by some of the following fitters; the default values will almost always suffice. The keywords FITACCURACY and MAXFUNCTIONS are used by all the fitters. A description of these minimizers follows:

1) LMCHOL - This is a minimizer that uses analytically computed gradients and makes specific use of the sum-of-squares property of the function that is being minimized. The analytic gradients are computed as the expectation value in the distorted waves of the derivatives of the potential. The potential derivatives are evaluated numerically. LMCHOL is based on the Harwell subroutine VA07A which was coded by Fletcher. Despite the fact that the computation of the gradients can more than double the chi-squared sum evaluation time, the LMCHOL and QUAVER fitters usually find a minimum in less than half the CPU time required by the other fitters. We know of no cases inwhich the CPU time is significantly longer for LMCHOL. The LMCHOL fitter is therefore highly recommended and is the default fitter.

2) QUAVER - This is a quasi-Newton fitter that uses a pseudo-inverse procedure to solve the required systems of linear equations. The search path followed by QUAVER differs significantly from that followed by LMCHOL only when there are directions in parameter space for which the second derivative of chi-squared is nearly zero. The keyword FITRATIO may be used to eliminate steps along such poorly determined linear combinations of the optical model parameters. The default value of 10^{-4} will have this effect; smaller values (such as 10^{-15}) will eliminate such restrictions on the search direction, and result in searches that are almost identical to those of LMCHOL. Setting PRINT=2 (page 80) will cause the singular values (the quantities that indicate which linear combinations of parameters are poorly determined) to be printed at each iteration. For both the QUAVER and MINIM fitters, the keyword FITMULTIPLE is a divisor used to reduce the step length when a step to a larger function value is attempted. The default value is 5.

3) MINIM - This is a variable-metric fitter using the 1972 Fletcher presciption for the metric update. It is generally slower than the above two fitters.

4) DAVIDON - This uses the original variable-metric prescription of Davidon. It is based on the Davidon fitter found in the Argonne Applied Mathematics Division library. This fitter is somewhat slower than the Fletcher fitter (MINIM). The keyword FITMULTIPLE determines the initial estimate of the metric matrix. The default (FITMULTIPLE = 0 or FITMULTIPLE > 100) is to use the second derivative approximation generated from the Jacobian of the chi-squared function. If FITMULTIPLE is set to a nonzero value, a diagonal matrix will be used as the initial metric and thus the search will start along the gradient direction. The diagonal elements of the matrix will be |FITMULTIPLE|*D(i) where D(i) = 1 if FITMULTIPLE > 0, and D(i) = x(i)**2 if FITMULTIPLE < 0 (x designates the parameter vector). The keyword NUMRANDOM may be used to specify the number of random steps that are to be made in confirming a minimum. The default is zero.

5) POWELL65 - This is a minimizer that makes specific use of the sum-of-squares property of the function but does not require Ptolemy to evaluate the gradient of the function. It is the Harwell subroutine VA02A which is based on a 1965 paper of Powell. The POWELL65 search algorithm is usually quite efficient for the first few iterations but then often begins to take very small steps for subsequent iterations. Therefore it often pays to terminate the search intermittently and restart it again. This may be accomplished by using the keyword REINITIALIZE to specify the number of iterations between restarts. REINITIALIZE = 16 is a reasonable value for POWELL65; the default is zero which suppresses reinitialization. The keyword FITMULTIPLE is used to limit the size of a single step; no step will be allowed to exceed FITMULTIPLE*FITACCURACY in relative size. The default is 500, but some tests indicate that larger values (10000) may result in faster searches.

6) ROCORD - This minimizer does not make use of the sum-of-squares property of the function nor of derivatives. It is provided as an alternative should the preceding minimizers fail to behave reasonably. The keyword FITMODE may be used to specify the initial value of IRET for ROCORD; the default is -1021, and should be adequate for most purposes. The keyword NUMRANDOM has the same meaning as for the DAVIDON fitter.

The FITACCURACY keyword may be used to specify the accuracy with which the potential parameters are to be found. Its significance depends upon which minimizer is used but for the first five fitters above it gives the relative accuracy to which each potential parameter or the minimum chi-squared value is to be found. The default value is 10^{-3}. This keyword is set by the elastic

PARAMETERSET's (page 40). The MAXFUNCTION keyword limits the number of chi-squared sums that may be evaluated during a search. Its default value is 50 which is more than enough for the default fitter (LMCHOL).

C - Reading the Output

The output for an optical-model fit begins with a summary of the elastic channels that are being fitted. For each data group, the laboratory energy, the CHANNEL specification, and the type of statistics are listed. The orbital angular momentum range and the stepsize used in solving the Schroedinger equation are also printed. This information is followed by a list of the parameters that are being varied in the fit and their initial values. If data was entered in the laboratory system, the conversion of that data to the c.m. system is shown next. In all subsequent output, the data and fitted values will be printed in the c.m. system only.

One or more pages is then produced for each data group showing the initial values of the fit. The potential parameters evaluated for the channel and laboratory energy are given for each data group. These are followed by a tabulation of the experimental and computed values of the cross sections at each angle involved in the fit. The cross sections are given as ratios to the Rutherford cross section and the angles are c.m. angles. The unsquared contributions to the chi-squared sum are given in a column labeled "(FIT-EXP)/ERROR;" the chi-squared sum is the sum of the squares of the entries in this column. The factor WEIGHT is not included in this column. The last column in this tabulation is labeled "%/L AT LMAX" and has been described in Sec. IV-E. Each data group listing is terminated with several lines summarizing the chi-squared for that group. The first line gives the chi-squared per point (both unweighted and weighted) computed using the RENORMALIZATION entered by the user (the value is also printed in the line). The next line gives that value of RENORMALIZATION that results in the minimum chi-squared (assuming that no other parameters are changed) and the resulting unweighted chi-squared per point. Finally, if there is more than one data group in the fit, the contribution of the current group to the total weighted chi-squared per point is printed, and the total chi-squared per point and chi-squared per degree of freedom for all the data groups are listed at the end of all the data groups.

After this listing of the initial conditions, the course of the fit is summarized by several lines printed at the end of each iteration. The lines give the total chi-squared per point and the corresponding parameter values (the parameters are listed in the order they were specified in the FIT keyword — this order may be found in the top right-side of the header on each page). If the listing of iterations terminates with the message

FIT COMPLETE. FINAL RESULTS FOLLOW

then the minimizer being used located a minimum of chi-squared and terminated normally. Any other message indicates an abnormal termination. The most likely cause of an abnormal termination is the failure of the minimizer to locate a minimum within the allowed number of function references (steps); such a condition is indicated by the message

NOT ENOUGH ITERATIONS TO ACHIEVE A GOOD FIT

In such cases the parameter values at the time of termination of the minimizer are used as the final parameter values; <u>these will not be parameters corresponding to a minimum of chi-squared</u>. Ptolemy then gives a listing of the final parameter values and of the resulting fit; the format of this listing is identical to that used for the initial conditions.

A page labeled "FINAL VALUES AND UNCERTAINTIES" follows the listing of the fit. This page has a column for each fit parameter; the columns are labeled with the parameter names. The first line of the table contains the final value of each parameter. Next are several lines giving the gradient at the minimum; the gradient is ideally zero but if there are large second derivatives may be significantly non-zero. Then there are two lines giving the RMS uncertainty and the relative RMS uncertainty in the parameters. These are based on the diagonal elements of the covariance matrix (error matrix) and are defined as the changes in the parameter values that would result in the chi-squared (not chi-squared per point) increasing by unity. Finally the eigenvalues and eigenvectors of the relative covariance matrix are listed. Each row of this listing contains the square root of an eigenvalue and the corresponding eigenvector. The square root of the eigenvalue is the relative change in the linear combination of parameters specified by the eigenvector that would result in the chi-squared increasing by unity. Thus eigenvectors with small eigenvalues represent well-determined combinations of parameters.

VI - Collective Model DWBA for Inelastic Excitation

Ptolemy is capable of doing DWBA calculations for inelastic-scattering reactions. The collective-model form factor is used for the nuclear part of the effective interaction. Only one nucleus may be excited in the reaction and that nucleus must initially have spin zero. The multipolarity (refered to as Lx) of the excitation must be greater than zero, but is otherwise not limited. The effective interaction that causes the excitation is the radial derivative of the Coulomb and both real and imaginary nuclear parts of an optical potential. Usually this optical potential will be that of the incoming channel, but a different potential may be used.

A - Specifying the Physical Problem

In a standard Ptolemy calculation of an inelastic-scattering reaction, the input will be in the following order:

1) Masses, charges, etc., of the 4 nuclei.
2) Grid and other calculation-control parameters.
3) Optical potentials for the two scattering states.
4) Optional potential changes for effective interaction.

Variations of this order are possible: item 4) is not required and item 2) may be spread among the other items.

In more detail a typical Ptolemy input deck for inelastic excitation will look like

```
REACTION:  reaction definition, ELAB = ...
PARAMETERSET ...., other parameter specifications
INCOMING      incoming optical parameters  ;
OUTGOING      outgoing optical parameters  ;
Effective-interaction parameters (optional)
;
RETURN
```

Here the keywords INCOMING, and OUTGOING indicate which potential parameters are being entered. The semicolons indicate that the complete potential has been defined and that Ptolemy is to go ahead with that stage of the computation (the semicolons are actually part of the input). The final semicolon indicates that all of the computational parameters have been entered and that the DWBA calculation should begin. Of course each of the potential specifications will in general require more than one input line.

The easiest way to define the participants in the reaction is to use the REACTION keyword. This keyword is followed by the statement of the reaction in standard nuclear terminology. Some examples will best illustrate the possibilities:

```
REACTION:  48CA(C12, 12C)CA48(2+ 3.83)
REACTION = 208PB(160, 160(6.13, 3-))208PB
```

All four nuclei must be included in the REACTION specification, and the complete reaction specification must be on the same input line as the REACTION keyword. Excited state information is enclosed in parentheses with no spaces or other punctuation separating the nuclear symbol and the left parenthesis. Except as has been otherwise indicated, blank spaces and commas may be freely used to make the reaction specification more readable. See the description of the CHANNEL keyword (page 33) for details concerning the nuclide symbols and excited-state specifications.

The REACTION keyword results in the definition of the atomic mass, charge, spin, and excitation energy of the four particles. Individual data values defined by the REACTION keyword may be overriden by the use of other keywords or the REACTION keyword may be omitted and all of the particle definitions entered via other keywords. These keywords are described in the chapter on transfer reactions (page 62).

The scattering energy is entered by either of the keywords ELAB or ECM followed by the energy in MeV. In both cases the energy refers to the incident kinetic energy; the outgoing energy is determined from the Q value of the reaction. The excitation energy is normally used by Ptolemy to determine the Q value of the reaction. If desired, a different Q value may be entered by using the keyword Q followed by the value in MeV.

The optical potentials for incoming and outgoing states are entered using the potential defining keywords of Sec. IV-B. The keywords INCOMING and OUTGOING indicate which state is being defined and a semicolon (;) is used to indicate the end of a particular definition. There are no default values for the radius or diffusness parameters. The well depths are all zero by default. The potential parameters used for the incoming state will also be used for the outgoing state unless they are explicitly overriden. The laboratory energy corresponding to the outgoing scattering energy is used for the outgoing scattering parameters so that the same keyword values will give slightly different potentials in the incoming and outgoing channels if an energy dependence is specified. As an example, the input lines

```
INCOMING  V=50  VI=25  R0=1.2  A=.5  RC0=1.2  ;
OUTGOING ;
```

define the same optical potential for both the incoming and outgoing states. Since the radius and diffuseness of the imaginary potential are not given, they are choosen to be the same as those of the real potential.

At present spin-orbit forces may not be used in the scattering states of DWBA calculations.

The effective interaction for the inelastic excitation is:

```
H(r) = -BETA * [ R'*d(Vreal)/dr + RI'*d(Vimag)/dr ]
     + BETAC*RC' * 3ZA*ZBIGA*e²/(2Lx+1) * f(r)     ,
```

where

```
f(r) = r**Lx / RC**(Lx+2)              r < RC ,
     = RC**(Lx-1) / r**(Lx+1)          r ≥ RC .
```

Here R' is the nuclear radius of the nucleus that is being excited:

```
R'  = R0  * A'**(1/3)
RI' = RI0 * A'**(1/3)
RC' = RC0 * A'**(1/3)
```

where the R0 are the radius parameters used in the effective interaction. The atomic weight of the excited nucleus is denoted by A' (A' = MA or A' = MBIGA). The quantities BETA*R', BETA*RI', and BETAC*RC' are the so-called deformation lengths of the excited nucleus. The definition of f(r) is that obtained from a multipole expansion of a point charge interacting with a uniform sphere of charge. Note that the full RC (not RC') appears in f(r).

The dimensionless Coulomb and nuclear deformation parameters may be entered with the keywords BETAC and BETA respectively. Alternatively the Coulomb deformation may be specified by the keyword BELX which enters the B(E, Lx), in units of e²barn**Lx, for the corresponding electromagnetic <u>excitation</u> process:

```
BELX = B(E, excitation)                                   ,
     = [2J(final)+1]/[2J(initial)+1] B(E, decay) .
```

The value of BETAC is then computed from

```
BETAC = 4*Pi/(3*Z) * sqrt(BELX) * (10/RC')**Lx
      * sqrt{[2J(initial)+1][2Lx+1]/[2J(final)+1]} ,
```

where Z is the atomic number of the excited nucleus and RC' (in fm) is defined above. If both BETA and BETAC (or BELX) are not specified, then the missing parameter is chosen such that the deformation lengths are equal:

```
BETA*R' = BETAC*RC' ,
```

where R' is the nuclear radius of the excited nucleus.

The optical potential that appears in the effective interaction is the optical potential that was used in the incoming state. It may be modified by entering different potential parameters after the semicolon that defines the outgoing state. If a potential parameter is not so changed, its value in the incoming state will be used. Thus

```
INCOMING  V=50  VI=20  R0=1.2  A=.65  RC0=1.2 ;
OUTGOING ;
VI = 1E-6 ;
```

will result in the effective interaction being essentially real. (Note that it is unfortunately not possible to redefine the well depths to be exactly zero.)

B - Controlling the Calculation

The keywords LMIN and LMAX, or LMINMULT, LMINSUB, LMAXMULT, and LMAXADD determine the range of L-values for which both the nuclear and Coulomb excitation amplitudes are computed. These keywords are explained on page 38, and reasonable values may be found in Table II below. The Lcritical used in the formulas on page 38 is the average of the critical L-values in the incoming and outgoing channels.

The Coulomb excitation amplitudes generally must be found for much larger values of L than the LMAX used for the nuclear amplitudes. Using a semi-classical approximation+, Ptolemy estimates an Lmax' such that the Coulomb amplitudes are negligible. The keyword DWCUTOFF may be used to control this choice; the choice is made such that

|Amplitude(Lmax')| = DWCUTOFF * |Amplitude(Lcritical)| ,

where both amplitudes are the pure Coulomb amplitudes. Pure Coulomb excitation amplitudes (evaluated using Coulomb scattering wavefunctions) are used for LMAX < L ≤ Lmax'.

For LMIN ≤ L ≤ LMAX, the nuclear and Coulomb amplitudes are evaluated as a one-dimensional integral over the range SUMMIN ≤ r ≤ SUMMAX. The Coulomb contribution for SUMMAX ≤ r < infinity is then evaluated using the asymptotic expansion described later. The lower limit (SUMMIN) is usually picked as that value of the radial coordinate beyond which the elastic scattering wavefunction for LMIN exceeds 10^{-15} in magnitude. The upper limit (SUMMAX) is

---

+ K. Alder, A. Bohr, T. Huss, B. Mottelson and A. Winther, Rev. Mod. Phys. 28, 432 (1956), Eq II E.83.

chosen to be the value of ASYMPTOPIA specified for the scattering wavefunctions. These two choices may be overridden with the keywords SUMMIN and SUMMAX, but there should be no need to do so. The number of Gauss points used in the one-dimensional integral is specified by the keyword SUMPOINTS which gives the number of points to use per average wavelength in the incoming and outgoing channels. SUMPOINTS does not need to be an integer. The Gauss points are mapped into the interval (SUMMIN, SUMMAX) using mappings defined on page 66 which are controlled by the keywords MAPSUM, GAMMASUM, and SUMMID. The default value of SUMMID is the midpoint of the (SUMMIN, SUMMAX) interval. There should never be any need to override the default mapping procedure.

The computation outlined in the previous paragraph leaves the following Coulomb excitation integrals to be evaluated:

1) Lmin $\le$ L $\le$ Lmax , SUMMAX $\le$ r < infinity ;
2) Lmax < L $\le$ Lmax' , 0 $\le$ r < infinity .

In case 1) it is necessary to do these integrals for both the regular and irregular Coulomb wavefunctions; linear combinations, based on the elastic incoming and outgoing S-matrix elements, of the resulting amplitudes are then used. For case 2) we assume that the scattering is determined by the point Coulomb charges alone and only the regular Coulomb wavefunctions are used.

In both cases the required Coulomb excitation amplitudes are found by recursion relations on L. These recursion relations are quite fast and are reasonably stable. The starting values of the recursion relations are found by a combination of numerical integrations and an asymptotic expansion+ for integrals of Coulomb wavefunctions and inverse powers of r. The numerical integrals are done cycle by cycle until the asymptotic expansion may be used; the number (which must be an integer) of Gauss points used in each wavelength is entered using the keyword NPCOULOMB. The relative accuracy required of the asymptotic expansion may be controlled by the keyword INELASACC. In addition a test of the recursion relations is made by explicitly computing the final recursed values. If the recursion relation is in error by more than 10*INELASACC, a warning message is printed. Reasonable values of NPCOULOMB and INELASACC may be found in Table II below.

The computation of the scattering wavefunctions may be controlled with the ASYMPTOPIA and STEPSIZE or STEPSPER keywords. These keywords are defined on page 39. As has just been described, the nuclear part of the excitation amplitude is integrated out to ASYMPTOPIA; by the use of the asymptotic Belling expansion, the Coulomb excitation amplitude is integrated to infinity.

+ J. A. Belling, J. Phys. B 1, 136 (1968).

The keyword PARAMETERSET (page 40) may be used to select standard groups of grid-setting parameters. Table II gives the PARAMETERSET names and the associated values that are suitable for

TABLE II
PARAMETERSET names and associated values for inelastic scattering calculations. The first column gives the default values.

Keyword	Default	INELOCA1	INELOCA2	INELOCA3
LMINMULT	.6	0	0	0
LMAXADD	30	20	30	50
LMAXMULT	1.6	1.6	2	2.6
SUMPOINTS	6	6	8	12
GAMMASUM	5	5	5	5
INELASACC	10^{-5}	10^{-3}	10^{-4}	10^{-6}
DWCUTOFF	10^{-3}	10^{-3}	10^{-4}	10^{-5}
NPCOULOMB	8	6	8	10
ASYMPTOPIA	20	20	25	30
STEPSPER	none	15	20	25

inelastic excitation calculations. Since the PARAMETERSET groups of Table II define values of ASYMPTOPIA and STEPSPER that are to be used in the two-body states, the PARAMETERSET keyword should precede the definitions of the two-body states.

C - Reading the Output

As each of the two scattering states are entered, a summary of the two-body channel and the potential is printed; this summary was described in Sec. IV-E. The computation of the inelastic excitation amplitudes is preceded by a page summarizing the reaction. This page contains a listing of the nuclei involved in the reaction, the deformation parameters, and the potential parameters used for the effective interaction. The column labeled "DEPTH" in the latter contains -3*ZA*ZBIGA*e² for the Coulomb part of the effective interaction. Next the range of angular momenta (LMIN, LMAX) for which both the nuclear and Coulomb amplitudes are computed is listed. This is followed with a summary of the one-dimensional integration grid that is used to compute the non-asymptotic part of these amplitudes.

Next a summary of the determination of the maximum L value (Lmax') needed for the Coulomb amplitudes is given. The maximum value required for each (Lx, Lout-Li) pair is given; the maximum of all of these values is then used. Following this summary one or more warning messages of the form

FOR LIN, LOUT = ... RECURSION IS POOR: .....

may be printed. These indicate that the recursed values of the Coulomb amplitudes did not compare well with the explicitly computed values. Both values are printed in the message. If the difference of the two values is not large, or if the values are both unusually small, then the message may be ignored. Otherwise the calculation should be repeated using a larger value of NPCOULOMB and/or a smaller value of INELASACC. A page labeled "INTERPOLATION AND EXTRAPOLATION IN L" contains the line "MAXIMUM LO USED IN COMPUTING ...". This line gives the maximum value of L (Lmax') for which the Coulomb amplitudes were computed by the recursion relations.

The pages labeled "REACTION AND ELASTIC PARTIAL WAVE AMPLITUDES" give the amplitudes for LMIN ≤ L ≤ LMAX. The columns labeled "RADIAL INTEGRAL" give the magnitude and phase (in radians) of the inelastic excitation amplitude. This is the amplitude defined in Eq. (II.39) except that a factor (BETA+BETAC)/2 has been removed. The columns labeled "INCOMING ELASTIC" and "OUTGOING ELASTIC" give the magnitudes and phase-shifts (in radians) of the elastic S-matrix elements. The Coulomb phase shifts are also given in radians.

The last set of pages give the inelastic excitation cross sections. These are given (in millibarns) in a column labeled "REACTION" and are c.m. values. The column labeled "LOW L %/L" has the significance described in Sec. IV-E, however the column labeled "% FROM L > LMAX" has a quite different meaning from the corresponding column in the elastic scattering output. Here the column gives (as a percentage) the total contribution of the (pure Coulomb) amplitudes for LMAX < L ≤ Lmax'. It is not to be construed as an indication of error. The columns labeled "INCOMING/RUTHERFORD" and "OUTGOING/RUTHERFORD" give the elastic cross sections relative to the Rutherford values.

Following the tabulation of the differential cross sections is a line labeled "TOTAL." This line gives the total inelastic excitation cross section (computed by summing the partial-wave amplitudes — not by integrating the printed angular distribution) and the total reaction cross sections for the entrance and exit channels. Following this line is a breakdown of the total excitation cross section into contributions from each magnetic substate (the axis of quantization is the incoming beam direction). Although values are listed only for Mx ≥ 0, the listed values for Mx > 0 are not doubled.

VII - Finite Range DWBA for Transfer Reactions

Ptolemy can carry out finite range DWBA calculations for particle transfer reactions. The reaction may be either stripping or pickup, and may involve more than one exchanged orbital angular momentum (refered to as Lx). Either the post or prior approximation may be used, and the effective interaction may include terms for the Coulomb part of the bound-state potential, the core-core Coulomb optical potential, and the real part of the core-core nuclear optical potential. When all these terms are included, the descrepency between post and prior calculations is usually less than a few percent. Core-core terms for the imaginary part of the optical potential may not be included.

A - Specifying the Physical Problem

In a standard Ptolemy calculation of transfer reactions, the input will be in the following order:

1) Masses, charges, etc., of the 5 particles.
2) Integration grid specifications and L-value ranges.
3) Potentials for the two bound states.
4) Optical potentials for the two scattering states.

Variations on this order are possible; the most likely is the spreading of item 2) amoung the other items.

In more detail a typical Ptolemy input deck will look like

```
REACTION:  reaction definition, ELAB = ...
PARAMETERSET ...., other computation parameters
PROJECTILE   projectile bound state parameters ;
TARGET       target bound state parameters ;
INCOMING     incoming optical parameters  ;
OUTGOING     outgoing optical parameters  ;
;
RETURN
```

Here the keywords PROJECTILE, TARGET, INCOMING, and OUTGOING indicate which potential parameters are being entered. The semicolons indicate that the complete potential has been defined and that Ptolemy is to go ahead with that stage of the computation (the semicolons are actually part of the input). The final semicolon indicates that all of the computational parameters have been entered and that the DWBA calculation should begin. Of course each of the potential specifications will in general require more than one input line.

The easiest way to define the participants in the reaction is to use the REACTION keyword. This keyword is followed by the statement of the reaction in standard nuclear terminology. Some examples will best illustrate the possibilities:

```
REACTION:  48CA(160, 14C)50TI
REACTION = 208PB(O16,15N)BI209(7/2- .90)
REACTION   PB208(O16 15N(3/2, 6.3239))BI209
REACTION   PB208(160(2,6.93) 12C)PO212
```

All four nuclei must be included in the REACTION specification, and the complete reaction specification must be on the same input line as the REACTION keyword. Excited state information is enclosed in parentheses with no spaces or other punctuation separating the nuclear symbol and the left parenthesis. An excited state of the initial target may <u>not</u> be given in this manner, but any or all of the other three particles may have excited state descriptors. See the description of the CHANNEL keyword (page 33) for details concerning the nucleid symbols and excited-state specifications. Except as has been otherwise indicated, blank spaces and commas may be freely used to make the reaction specification more readable.

The REACTION keyword results in the definition of the atomic mass and charge of the four particles. The atomic mass and charge of the exchanged particle is then computed by subtraction. The 1975 Oak Ridge Atomic Mass Adjustment and the 1971 Nuclear Wallet Cards compilation+ is then used to find the ground state mass excesses and spins of all 5 particles. The ground state mass excesses (along with the excitation energies, if given) will be used during the bound state computation to find the separation energies of the exchanged particle (X) from the appropriate cores.

Individual data values defined by the REACTION keyword may be overriden by the use of other keywords or the REACTION keyword may be omitted and all of the particle definitions entered via other keywords. The keywords that define the five particles have the form "Ki" where "K" indicates what quantity is being defined and "i" is a suffix indicating which particle is involved (BIGA, A, B, BIGB, or X). The possibilities for K are

M - The mass in AMU. This need not be an integer.
Z - The charge.
J - The spin of the nucleus.
MXCG - The mass excess of the ground state.
E* - The excitation energy in MeV.
MXC - The mass excess of the nucleus (MXCi = MXCGi + E*i).

+ F. Serduke, "Atomic Mass Table," Argonne Internal Report, 1975, and private communication.

As an example

MB=15, ZB=7, JB=3/2, E*B=6.3239, MXCGB = .10152

would define the excited state of ^{15}N contained in the third REACTION example given above. (Alternatively one could have entered MXCB = 6.42542 and left out the E*B and MXCGB keywords or one could directly enter the proton separation energy at the time of the ^{16}O bound state calculation and leave out all the mass excess specifications.) In the following example

REACTION: 209BI(16O 12C)213AT, JBIGB = 9/2

one is supplying the ground state spin of ^{213}At which is not in the the Nuclear Wallet Cards.

The scattering energy is entered by either of the keywords ELAB or ECM followed by the energy in MeV. In both cases the energy refers to the incident kinetic energy; the outgoing energy is determined from the Q value of the reaction.

The Q value may be entered by using the keyword Q followed by the value in MeV. If it is not entered it will be found as the difference of the two bound state energies. If it is entered then it is necessary to define only one of the bound state energies; the other will be found using the Q value. Since the REACTION keyword results in the definition of both bound state energies, it is usually not necessary to enter the Q value.

The version of the DWBA on which Ptolemy is based uses as the effective interaction that induces transfer the potential that binds the composite particle at either the projectile or target vertex. The vertex whose potential is to be used as the effective interaction is specified by the keywords USEPROJECTILE or USETARGET. USEPROJECTILE indicates that the potential for the projectile bound state is the interaction potential; USETARGET causes the target potential to be used. The default is USEPROJECTILE. Note that we avoid the use of the words "post" and "prior" in specifying the interaction vertex.

The content of the interaction potential is controlled with the NUCONLY, USESIMPCOULOMB, USECOULOMB or USECORE keywords. NUCONLY means that only the nuclear part of the bound state potential is used in the interaction potential. (Most published DWBA calculations have used this prescription). USESIMPCOULOMB means that the full bound state potential at the vertex designated by USEPROJECTILE or USETARGET is used. USECOULOMB causes the nuclear potential at the designated vertex to be used with the complete three-body Coulomb potential. The inclusion of the Coulomb corrections due to the third particle removes post/prior descrepancies from the Coulomb part of the interaction and can result in much closer agreement between USETARGET and USEPROJECTILE results. The keyword USECORE may be used to include both the Coulomb and core-

Coulomb corrections that are included by the USECOULOMB keyword and the core corrections from the real part of the nuclear optical potential. Core corrections due to the imaginary part of the optical potential (which are typically only a few percent) cannot be included. The default is USECORE. Note that DWBA calculations are usually somewhat simpler numerically if the interaction is attached to the vertex (usually the projectile vertex) involving the lighter ions. In a reaction such as ^{208}Pb(^{16}O, ^{17}O)^{207}Pb inwhich the projectile and target differ significantly in mass, a USETARGET calculation requires a substantially denser integration grid than is required for USEPROJECTILE, however if the USECORE option is selected, essentially the same cross sections will be found in both cases.

The spectroscopic amplitudes for the two bound states may be entered with the keywords SPAMP and SPAMT. These amplitudes will be squared and multiplied into the cross sections. The default values are unity. Alternatively the spectroscopic factors (the squares of the amplitudes) may be directly entered using the keywords SPFACP and SPFACT. The spectroscopic factors must be positive.

Potential parameters must be entered for each of the two bound states and the two scattering states. The potentials are defined when the bound state or scattering state is to be computed; the same keywords are reused to define the potentials in each of the four states. Each of these four two-body states consists of two particles that are referred to as the "projectile" and "target" (not to be confused with the projectile bound state and target bound state). In the scattering states these words have their normal meanings; for the bound states the exchanged particle (X) is always the "projectile". The potential parameters are defined in Sec. IV-B. The laboratory energy corresponding to the outgoing scattering energy is used for the outgoing potential parameters so that the same keyword values will give slightly different potentials in the incoming and outgoing channels if an energy dependance is specified.

If a given V or TAU is defined in a channel, then its associated R (or R0) and A must also be defined. At the beginning of input for each channel, all V's and TAU's are set to 0 and all R's and A's are undefined. However, potential parameters will be retained (if they are not overriden) from one bound state to the other and from one scattering state to the other. They will not be retained from bound states to scattering states or vice-versa. The same rules apply to RC and RC0, one of which must be defined for the bound states if both Zp and Zt are nonzero. If both RC and RC0 are undefined for the scattering states, the Coulomb potential of two uniform spheres (page 36) will be used.

At present spin-orbit forces may not be used in the scattering states of DWBA calculations.

Normally the binding energy (cluster separation energy) of the bound states will be computed by Ptolemy from the information in the REACTION specification. If it is desired to override this bound state energy, one may use the "E" keyword to enter the bound state energy along with the bound state potential. The energy is given in MeV and must be negative for bound states. The "E" keyword may also be used in the scattering state descriptions in which case it specifies the c.m. energy of the state. It will then override the c.m. energy determined from the ELAB keyword or from ELAB combined with the Q value depending on the channel. One may use the E*P or E*T keywords to enter the excitation energy of the projectile or target. Use of FITE (page 38) in DWBA calculations may result in bound state energies (and hence Q-values) that are significantly different from the values determined from the REACTION specification. The default is FITV.

B - The Integration Grid

The Ptolemy integration grid is constructed by a rather elaborate set of subroutines consisting of some 1100 Fortran source cards. The construction is fairly automatic and is designed to place the integration points where the integrand is largest. Ideally the user would not have to intervene in this process and would only have to tell the processor the desired accuracy of the final results (the differential cross sections). Unfortunately the subroutine is less than perfect and the user must have some understanding of what the subroutine does. This section describes most of the parameters that control the grid construction. The novice user of Ptolemy need not be concerned with the details of this section since the PARAMETERSET keyword described in the following section can be used to choose complete sets of grid-construction parameters. As is described in the following section, these parameters have been tuned for specific types of calculations; they may not be adequate for quite different types of calculations, and the convergence of the computed cross sections should be checked by repeating such calculations with a different set of parameters.

The Ptolemy integration grid is based on the three variables DIF, SUM, and PHI:

DIF = Ri - Rout ,
SUM = (Ri + Rout)/2 ,
PHI = angle between Ri and Rout.

Here Ri and Rout are the radial variables in the incoming and outgoing elastic channels. The form factor is first integrated over PHI. This results in a quantity that, for fixed values of DIF, is a smoothly varying function of SUM. However the scattering wavefunctions are often rapidly varying functions of SUM. Therefore the form factor is computed on a rather coarse grid of SUM values and interpolated to a fine grid for integration with the scattering wavefunctions. The numbers of points in each of the grids on which the form factor is computed are specified by the keywords NPSUM, NPDIF, and NPPHI, respectively. These numbers may have any value between 1 and 2000; typical values will be found in Table III below. The number of points in the SUM integration grid is specified by the keyword SUMPOINTS which gives the number of points per average wavelength in the entrance and exit channel. In this manner, the grid automatically becomes denser as the bombarding energy is increased; it is our experience that the other three grids (controlled by NPDIF, NPSUM and NPPHI) need not become denser as the bombarding energy increases. The same three-dimensional grid is used for all values of Li, Lout and Lx.

The keyword DWCUTOFF is used in the construction of the integration grids. DWCUTOFF specifies in a relative sense the smallest integrand (Ri * scattering wave * bound state * potential * bound state * scattering wave * Rout) to include in the grid. If the integrand at a point (Ri,Rout,PHI) is smaller than DWCUTOFF times the largest value of the integrand encountered, that point will not be included in the grid.

The lower and upper limits of the SUM grid are determined as the values of SUM for which the integrand has fallen (in a relative sense) beneath DWCUTOFF at DIF = PHI = 0. The scattering wavefunctions for L = LMIN are used when finding the lower limit of SUM while the wavefunctions for L = Lcritical are used for the upper limit. These two limits may be overriden by using the SUMMIN and/or SUMMAX keywords to give values (in fm) of the lower and upper limits.

The SUM grid points are mapped into the interval (SUMMIN, SUMMAX) in a manner that clusters them about a "midpoint." This midpoint is at present chosen to be the expectation value of SUM (weighted by the integrand for L = Lcritical) for DIF = PHI = 0. The value of the "midpoint" may be overridden with the keyword SUMMID or it may be multiplied by a factor specified by the MIDMULT keyword, however the resulting value will always be constrained to be not greater than the average of SUMMIN and SUMMAX.

The form of mapping used for the SUM grid may be controlled by the MAPSUM keyword which may have one of the following values:

0 - linear mapping with no compression.
1 - cubic mapping with Sinh compression.
2 - rational mapping with Sinh compression (default).
3 - linear mapping with Sinh compression.

SUMMAP = 2 gives the best results in the cases so far examined and is the default. The degree of compression in mappings 1-3 is controlled by the GAMMASUM keyword. Suitable values are indicated in Table III below.

The DIF grid limits are determined by the values of DIF for which the form factor becomes smaller in a relative sense than DWCUTOFF. Initially these limits are chosen separately for each of the NPSUM values of SUM. Each DIF grid is also mapped about a "midpoint" which is chosen to be the location of the maximum of the form factor for the fixed value of SUM (and PHI = 0). Since the automatic choice of the DIF limits and midpoints seems always to be successful, no keywords are provided to override these values. The keyword MAPDIF is used to choose the DIF mapping and has the same meanings as the MAPSUM keyword. The best value in the cases studied is 1 which is the default. The keyword GAMMADIF specifies the degree of compression used in the mapping.

To allow interpolation in the SUM variable, the DIF grid points must be smoothly varying functions of SUM. The procedure outlined in the previous paragraph does not necessarily produce such a grid. Therefore low-order polynomials in SUM are fitted to the families of DIF points that are choosen above. These polynomials are then used to generate the DIF points that are actually used in the calculation. The order of these interpolating polynomials may be specified by the VPOLYORDER keyword; the default is 3 which is almost always adequate. (The error message

"INVALID VMIN, VMID, VMAX ...."

usually means that VPOLYORDER should be increased, although the cross section values are often only slightly affected by this error.)

The PHI maps are individually chosen for each value of SUM and DIF. The minimum PHI is always 0 and the maximum is determined as the point at which the form factor falls in a relative sense beneath DWCUTOFF. For heavy ion reactions this is usually a small angle [Cos(PHI) > .99]. The PHI map is a linear map in the variable Cos(PHI).

C - Controlling the Calculation

The keywords LMIN and LMAX, or LMINMULT, LMINSUB, LMAXMULT, and LMAXADD determin the range of L-values for which the transfer amplitudes are computed. These keywords are explained on page 38, and reasonable values may be found in Table III below. The Lcritical used in the formulas on page 38 is the average of the critical L-values in the incoming and outgoing channels.

Not all radial integrals used in computing the differential cross sections need be explicitly computed by Ptolemy. Ptolemy will interpolate between computed values and extrapolate beyond the largest value of L for which the radial integrals are computed. The keyword LSTEP determins which radial integrals are to be computed. The radial integrals for

Lout = LMIN, LMIN+LSTEP, LMIN+2*LSTEP, ...,

(where the sequence stops at or before LMAX) will be computed. The radial integrals for all Lx and Li associated with these Lout's will be computed. The remaining radial integrals for LMIN ≤ Lout ≤ LMAX will then be found by interpolation using continued fractions. The default value of LSTEP is 1 which causes all radial integrals from LMIN to LMAX to be computed explicitly.

In addition Ptolemy will pick an Lmax' > LMAX such that radial integrals for Li, Lout > Lmax' are negligible. The radial integrals for LMAX < Li, Lout ≤ Lmax' will be found by extrapolation. The extrapolating function used is of Woods-Saxon form in L. Thus LMAX must be sufficently beyond the L-window for such a shape to be an adequate representation of the radial integrals. The keyword MAXLEXTRAPOLATION may be used to limit or completely suppress the extrapolation to L > LMAX. It specifies the maximum allowed Lmax'-LMAX. If it is set to 0, no extrapolation will occur. The default value is 100.

Since no extrapolation to Li, Lout < LMIN is made, LMIN must be small enough to include all important radial integrals. Care should be taken to avoid specifying too small a value of LMIN since the radial integrals for small Li and Lout are small due to extensive cancellations of the integrand viewed as a function of Ri+Rout. In practice these cancellations are hard to reproduce without using a large number of Gauss points and the computed radial integrals may be much larger than they should be. Thus a more accurate solution is often obtained by totally excluding integrals whose contributions are very small but which are hard to calculate accurately.

For a given reaction there will usually be several possible values of the transfered orbital angular momentum:

Lx = Lout - Li = J(projectile) - J(target) .

Ptolemy will compute the radial integrals for all possible values cf Lx and add the resulting cross sections together with the appropriate Racah coefficients. If only one value of Lx is possible the resulting cross section will still be weighted by the Racah coefficient. If it is desired to have results for only one value of Lx, the keyword LX may be used to specify the desired value.

The computation of the two-body wavefunctions (both bound and scattering states) may be controlled with the ASYMPTOPIA and STEPSIZE or STEPSPER keywords. These keywords are defined on page 39. ASYMPTOPIA and STEPSIZE or STEPSPER may be respecified for each of the four two-particle states; if they are not reentered, the value last entered is used.

The value of ASYMPTOPIA in effect when the bound states are specified is the largest value of Rp or Rt (the radial coordinates of the projectile and target bound-state wavefunctions) at which the bound-state wave functions will be found and thus must be large enough to satisfy the needs of the integration grid. The largest values of Rp and Rt used by the integration grid are printed in the summary of the grid.

The largest value of Ri and Rout (the scattering variables) will automatically be chosen to be large enough to satisfy the needs of the integration grid. However it will never be smaller than the value of ASYMPTOPIA in effect at the time of input of the optical potentials. Therefor since, as has just been explained, a large ASYMPTOPIA is often needed for the bound-state wave functions, substantial core savings may be realized by reducing ASYMPTOPIA to as small a value as is physically reasonable for the scattering states; it will then be automatically increased to the required value.

The keyword PARAMETERSET (page 40) may be used to select standard groups of grid setting parameters. Table III gives the PARAMETERSET names and the associated values that are suitable for transfer calculations. Since the PARAMETERSET groups of Table III define values of ASYMPTOPIA and STEPSPER that are to be used in the two-body states, the PARAMETERSET keyword should precede the definitions of the two-body states. The CA60A and CA60B PARAMETERSET names are appropriate for two-nucleon transfer reactions initiated by ^{16}O on Ca near 60 MeV. The PB100A, PB100B, and PB100C PARAMETERSET names are designed for single-nucleon ^{16}O on Pb reactions near the Coulomb barrier; at bombarding energies of several hundred MeV, larger values of LSTEP may be used. The ALPHA1, ALPHA2 and ALPHA3 sets were designed for (^{16}O, ^{12}C) reactions on targets around ^{24}Mg.

Table III shows that as one increases the numbers of grid points, one should also reduce DWCUTOFF so as to include more of the integrand in the computation. This reduction in turn means that ASYMPTOPIA may have to be made larger. The larger intervals that result from the smaller DWCUTOFF will also result in the Gauss points being spread out further so that the same number of points will give reduced accuracy. The ALPHAi sets have significantly larger NPSUM and NPDIF values than the other sets. These are due to the facts that the alpha-core bound state wavefunctions have a large number of nodes, and that the DIF grids for alpha transfer extend further than for than for one- and two-nucleon transfer.

It is strongly suggested that for each substantially new problem, the user make calculations with several different sets of grid parameters to verify that convergence has been achieved. Many nodes in the bound-state wavefunctions, a strong dependence on L (such as is obtained with surface transparent potentials) of the elastic scattering wavefunctions, poorly matched reactions, and transfers of heavy clusters are all examples of cases in which modifications of the parameter sets may be necessary.

TABLE III

PARAMETERSET names and associated values for DWBA transfer calculations. The first column gives the default values.

Keyword	Default	CA60A	CA60B	PB100A	PB100B	PB100C
LSTEP	1	3	2	5	4	3
DWCUTOFF	10^{-3}	10^{-2}	10^{-3}	10^{-3}	$3*10^{-3}$	10^{-4}
SUMPOINTS	6.	6.	6.	2.5	3.	3.5
NPSUM	15	10	15	10	15	20
NPDIF	10	10	13	8	10	14
NPPHI	10	10	12	10	12	16
LMINSUB	20	10	15	12	16	20
LMINMULT	.6	.6	.5	.86	.78	.70
LMAXADD	30	15	20	30	35	40
LMAXMULT	1.6	1.5	1.7	1.6	1.8	2.0
GAMMASUM	5.	5.	5.	10^{-3}	10^{-3}	10^{-3}
GAMMADIF	5.	5.	5.	3.	3.	3.
ASYMPTOPIA	20	20	25	45	50	55
STEPSPER	none	12	20	8	12	16

Keyword	ALPHA1	ALPHA2	ALPHA3
LSTEP	2	1	1
DWCUTOFF	10^{-3}	10^{-4}	10^{-5}
SUMPOINTS	6.	7.	8.
NPSUM	40	50	70
NPDIF	25	30	35
NPPHI	12	14	16
LMINSUB	10	15	20
LMINMULT	.6	.5	.4
LMAXADD	15	20	25
LMAXMULT	1.5	1.7	2.0
GAMMASUM	3.	3.	3.
GAMMADIF	5.	5.	5.
ASYMPTOPIA	20	25	30
STEPSPER	12	20	25

D - Saving Time and Core with SAVEHS and USEHS

Almost all of the time in a large DWBA calculation is devoted to the form factor integral:

H(Ri,Rout) = Integral d(PHI) (B.S. Veff B.S.)

These quantities are independent of both the optical potentials and the scattering energy. Most DWBA studies are principally concerned with the effects of variations in the optical potentials. Thus it is reasonable to save the computed H's in a dataset for reuse with different optical potentials. If a study is being made at a number of relativly close energies, time can also be saved by making one large calculation containing all of the orbital angular momenta needed for all of the energies, and then in subsequent jobs using subsets of the resulting dataset. Ptolemy provides two keywords, SAVEHS and USEHS, to allow the form-factor integrals to be saved.

The SAVEHS keyword is used to initiate the saving of the integrals over PHI of the form factor. These integrals may then be reused in later calculations with different optical potentials at a considerable saving in CPU time. The SAVEHS keyword must be entered before the first semi-colon and should be entered after the HEADER and REACTION keywords if they are used. If SAVEHS is used the Fortran file (DD name) FT01F001 must be defined (see Appendix C).

The USEHS keyword is used to indicate that the H-integrals saved in a previous calculation with the SAVEHS keyword are to be reused. USEHS must be entered before the first semicolon. If it is used, the REACTION, LSTEP and all grid-setting keywords should not be specified again. The bound state potentials must not be entered; rather the definitions of the new optical potentials should directly follow the USEHS keyword. These definitions are then followed by the final semicolon indicating that the DWBA calculation is to begin. Thus a typical USEHS run has the form

```
USEHS
INCOMING  potential definition  ;
OUTGOING  potential definition  ;
;
RETURN
```

If ELAB, LMIN, and/or LMAX are not specified, the SAVEHS values will be used. However new values of these parameters may be specified in the USEHS run. If different values are to be specified; they must be given after the USEHS keyword. If a different LMIN is specified, the user must insure that it was one of the values explicitly computed in the SAVEHS run [i.e. that LMIN = LMIN(SAVEHS) + n*LSTEP]. If a new value of ELAB is specified, the SUM grid will not be the optimal grid since it was chosen for a different energy. In cases in which it is desired to do USEHS runs at different energies, the SAVEHS run should be made at the maximum energy to be used. It should be made with more SUM points than would be necessary for a calculation at a single energy. Also the automatic choice of LMIN will have to be reduced.

Since the large arrays used for the angular transforms in the form-factor integral do not need to be constructed for USEHS calculations, there are also substantial core savings in USEHS jobs.

All but the largest USEHS calculations can be made within the Argonne express limits of 250K and two minutes of /195 CPU and wait time. It is suggested that during a study of a given set of reactions, a SAVEHS run be made for each different reaction, and the results stored on the on-line disks. The effects of different optical potentials may then be quickly and cheaply studied for all the reactions using USEHS jobs. When the study is complete, the SAVEHS datasets may be copied to a tape for long-term storage.

E - Reading the Output

As each of the bound states and elastic scattering states are entered, a summary of the two-body channel is printed; the format of this summary has been described in Sec. IV-E. When the fifth semicolon is entered, a summary of the reaction is printed. This summary lists the nuclei involved, the bound-state properties, and the spectroscopic factors. The Q-value of the reaction is also printed. If the Q-value or the bound-state or outgoing scattering energies were explicitly entered by the user, then the differences of the bound-state energies and of the scattering energies may not be the same, or they may not be equal to the Q-value. Under these circumstances an appropriate warning message is printed, however the calculation proceeds with the bound-state and scattering energies that were listed in the previous summaries. After the bound-state properties, the content of the effective interaction, as determined by one of the keywords NUCONLY, USESIMPLECOUL, USECOULOMB, or USECORE, is listed.

The range of I's and the increment of L for which the radial integrals will be explicitly computed is then listed. The range of transfered orbital angular momenta is also given.

A several-line summary of the three-dimensional integration grid is then given. The lines give the number of Gauss points used for, and the extent of, each dimension of the grid. The entry under "NUM. PTS." for (RI+RO)/2 gives the number of Gauss points used in the integrals involving the wavefunctions, and is determined by the value of SUMPOINTS; the form factors are found at these points by interpolation. The number of points in the (RI+RO)/2 grid at which the form factors are evaluated (NPSUM) is given in parentheses at the end of the (RI+RO)/2 line. The warning message

INVALID VMIN, VMID, VMAX ...

may precede the integration grid summary; it is explained in Sec. VII-B. Two lines of the form

MAXIMUM R'S USED FOR ...

give the maximum radial coordinate values for which each of the bound-state and scattering-state wavefunctions will be used in the three-dimensional integrals. The corresponding values of ASYMPTOPIA may be reduced to approximately 5 fm greater than these values in future calculations. If the bound state ASYMPTOPIA prove to be limiting factors in the grid construction, the warning message

```
ERROR... BOUND STATE WAVEFUNCTIONS NEEDED ....
IN FUTURE RUNS INCREASE ASYMPTOPIA TO ....
```

will be printed. The calculation should be repeated with an increased value of ASYMPTOPIA for the bound states since the radial integrals computed with the smaller grid may not be accurate. The increased value should be at least 5 fm larger than the values printed in the warning message.

If (as is suggested) PRINT=2 has been specified, one or more pages labeled "COMPUTATION OF RADIAL INTEGRALS" will next be printed. These pages contain only those radial integrals that are explicitly computed; the radial integrals for even Lout are printed first. Three columns give the real and imaginary parts and the magnitude of the radial integrals. These are followed by two columns labeled "CANCELLATIONS;" the second of which is not presently used. The first column gives an indication of the numerical cancellations that occurred in the d(Ri) d(Ro) integral and is defined as

```
Integral d(Ri,Ro) Ri Ro | f(out) H f(in) | /
    | Integral d(Ri,Ro) Ri Ro f(out) H f(in) |
```

where the denominator is just the radial integral. The entries in this column are usually quite large (>100) for the smaller values of L, since these radial integrals are small by virtue of large cancellations. However the values for L ≥ Lcrit are usually less than 5, indicating that there was not much difficulty associated with these radial integrals. If all of the entries in this column are greater than 10, then the reaction is in some way poorly matched, and the convergence of the computed cross sections should be carefully checked.

The page labeled "INTERPOLATION AND EXTRAPOLATION IN L" gives a summary of the extrapolation of the radial integrals from LMAX to Lmax'. The value of Lmax' is printed in the line "MAXIMUM LO USED ...". This line may be preceded or followed by a number of warning or error messages indicating difficulties in the extrapolation to Lmax'. These difficulties are usually associated with the fact that some (Lx, Lin-Lout) combinations are poorly matched and the computed radial integrals contain large errors. If the errors are large enough, the computed radial integrals will not have the correct asymptotic form, and it will be impossible to fit the extrapolating function to them. If the extrapolated radial integrals will have a negligible effect on the computed differential cross sections, then these error messages may be ignored. An indication of this may be found in the table labeled "SUMMARY OF EXTRAPOLATION PARAMETERS" that is printed at the end of this page. The (Lx, Lin-Lout) combinations that could not be extrapolated have zeros in the columns that give the extrapolation parameters. The columns labeled "PEAK" give the Lout for which the radial integrals with the printed values of Lx and Lin-Lout have their maximum magnitude and that maximum magnitude. If the maximum magnitude is small compared to other maximum magnitudes, then the extrapolated values (which are usually at least a factor 10 smaller) are probably negligible and the failure to be able to extrapolate may be safely ignored.

The pages labeled "REACTION AND ELASTIC PARTIAL ..." give all of the radial integrals and the elastic S-matix elements for LMIN ≤ L ≤ LMAX. The format of these pages was explained in Sec. VI-C.

Finally the cross sections are given on the pages labeled "COMPUTATION OF CROSS SECTIONS." Most of the entries on these pages were also explained in Sec. VI-C, and only the differences will be given here. The column labeled "% FROM L > LMAX" gives (as a percentage) the contribution to the cross section from the radial integrals for LMAX < L ≤ Lmax'. Our experience is that this contribution is usually accurate to somewhat better than 10%. Thus if at a given angle the entry is 5%, one may assume that the extrapolation procedure introduced an error of less than 0.5% to the differential cross section. If more than one Lx can contribute to the reaction, there will be columns giving the differential cross section for each Lx; the cross section in the second column is the sum of these partial cross sections. Of course the spectroscopic factors are included in all cross sections.

VIII - Control Keywords

In this section we describe some of the control keywords that are available in Ptolemy. These keywords may generally be placed anywhere in the Ptolemy input and they usually cause some sort of immediate action; they are not followed by a semi-colon. These keywords are listed more or less in decreasing order of interest; all of them except RETURN are optional.

The RETURN keyword should be used as the last keyword in every Ptolemy job. It causes allocator statistics to be printed and then returns control to the operating system.

The HEADER keyword may be used to enter a header that will be printed on the top of most pages of the Ptolemy output. The header will consist of the remainder of the input line beginning with the first alphanumeric following the HEADER keyword. In addition the REACTION specification (if it is entered) and the laboratory energy will always be part of the header.

The KEEP keyword is used to keep Ptolemy results in a form suitable for later recovery with the Speakeasy KEPT command. A Speakeasy KEEP dataset must be allocated to the file (DD name) MYKEEP if the KEEP keyword is to be used. Appendix C shows the JCL required to make such a dataset and to include it in the Ptolemy job. KEEP must be followed by two names: the first is the Ptolemy name of the item to be kept and the second is the name under which it is to be saved in the dataset. This second name must be different from all other names already in the dataset or else the new object will replace the previously kept object. The following is a list of the Ptolemy names of the objects the user is most likely to want to keep:

ANGLEGRID - A 3-element array containing ANGLESTEP, ANGLEMIN and ANGLEMAX.

CROSSSEC - The differential cross section on the (ANGLEMIN, ANGLESTEP, ANGLEMAX) grid. For DWBA calculations this contains the reaction cross section. For stand-alone elastic scattering it contains the elastic differential cross sections. In both cases it is in mb/sr.

TORUTHERFORD - The ratio of the elastic scattering differential cross section to the Rutherford cross section. This array is produced only in stand-alone elastic scattering.

LXCROSSSECTION - A Num(angles) X Num(Lx) array containing the DWBA cross sections for each Lx (summed over Mx) at each angle.

MXCROSSSECTION - A Num(angles) X Num(Li,Lx) array containing the DWBA cross sections for each (Lx, Mx) at each angle. The order of the columns is

(Lx,Mx) = (Lxmin,0), (Lxmin,1), ..., (Lxmin,Lxmin), (Lxmin+1,0), ..., (Lxmax,Lxmax) .

This array is available to KEEP only if the keyword SAVEMXCROSS (see below) has been entered.

IMAG and IPHASE - The magnitude and phase of the radial integrals. These two objects are each Num(L) X Num(Li,Lx) arrays. The arrangement of the columns is such that I(Lx, Li, Lout) is indexed as IMAG(j,k) and IPHASE(j,k) with

j = Lout-LMIN+1
k = [(Lx+Lxmin+1)(Lx-Lxmin) + Lx+Li-Lout]/2 + 1

B - A Num(angles) X Num(Li,Lx) complex array containing the B(Lx, Mx, theta) of Eq II.xxx or II.56 for each (Lx,Mx) at each angle. The columns have the same order as for MXCROSSSECTION. This array is available for KEEP only if the SAVEB keyword (see below) has been entered.

SIN - The elastic S-matrix elements in the incoming channel.

SOUT - The elastic S-matrix elements in the outgoing channel.

WAVER, WAVEI - The real and imaginary parts of the most recently computed elastic scattering wavefunction.

PHIn - The n'th bound state wavefunction.

HEADER - A character array (up to 65 characters) containing the HEADER.

REACTION - A character array (up to 45 characters) containing the REACTION or CHANNEL specification.

ELAB - A scalar with the laboratory energy.

The following symbols were used in the above definitions of the objects for the KEEP command:

Lxmax	Maximum Lx (transfered L)
Lxmin	Minimum Lx
Num(angles)	Number of angles
Num(L)	Lmax'-LMIN+1
Num(Lx)	Lxmax-Lxmin+1
Num(Li,Lx)	[(Lxmax+Lxmin+2)(Lxmax-Lxmin+1)]/2 (This expression does not take into account abnormal parity restrictions but it is always the correct expression to use.)

The SAVEMXCROSS keyword may be entered to cause the DWBA cross sections for every (Lx, Mx) and angle to be saved. The SAVEB keyword may be entered to cause the B(Lx, Mx, theta) to be saved for every (Lx,Mx) and angle. The resulting objects (MXCROSSSECTION and B) may then be stored using the KEEP command. The defaults are NOSAVEMXCROSS and NOSAVEB.

The WRITENS command is an alternative method of storing objects that are in the Ptolemy allocator for use by other programs. The command is followed by the name or number of an object in the allocator. The object will be written on Fortran unit 15 using a (1X, 4G17.8) format. If this command is used, a DD card defining DD name FT15F001 to be a card-image dataset must be part of the JCL used to invoke Ptolemy. The names and structures of the available objects are given in the description of the KEEP command above, however two-dimensional objects will be written as the transpose of the Speakeasy formats given above.

The NEWPAGE keyword may be used to cause subsequent Ptolemy output to begin on a new page. It will probably be used only if several stand-alone two-body calculations are being done.

The KEYWORDS keyword may be used at any time to cause a listing of the current settings of all data-entering and option-choosing keywords. It is suggested that it be used at the end of all runs to provide a verification of the parameters and options in effect. The LISTKEYS keyword will list the names of all valid keywords. It is useful in TSO applications to check the spelling of a keyword.

The UNDEFINE keyword may be used to set the status of a keyword to "undefined." It is followed by the name of the keyword that is to be undefined. The most likely use of UNDEFINE is to undefine a potential radius (R, RI, etc.) during stand-alone calculations so that it will automatically be computed from the corresponding radius parameter (R0, RI0, etc.) the next time it is needed. One may also want to undefine STEPSPER after the use of PARAMETERSET, so that a specific STEPSIZE may be entered.

The NSCATALOG keyword may be used at any time to provide a list of the names and sizes of all currently defined objects in the allocator. It will also give the NSSTATUS output.

The NSSTATUS keyword will cause a short summary of the allocator status to be printed. This summary will show the allocator size, its current in-use size and the peak in-use size. This summary is automatically printed at the end of all Ptolemy jobs.

The SIZE keyword may be used to specify the size of the allocator (the Ptolemy work area). If the SIZE value is given as a positive number, it is the size in bytes of the allocator. It is usually more convenient to enter a negative number which is interpreted as the number of bytes of core to leave for other purposes (such as I/O buffers); the remainder of the available core is used for the allocator. The default value of SIZE is -5000. This default is generally adequate but may be made closer to zero if no KEEP operations are anticipated. If it is to be used, the SIZE keyword should be on the first line of Ptolemy input.

The DUMP or NSDUMP keywords may be used to print an object in the allocator. They are followed by the name or number of the object to be printed.

The RESET keyword may be used to cause Ptolemy to be set back to its initial status. The complete allocator is cleared and all keywords are set to their default values. However the allocator size may not be changed after a RESET. The use of RESET allows several independent calculations to be made in one job. If it is desired to do a SAVEHS calculation and immediately follow it with several USEHS calculations, each USEHS step should be preceded with a RESET.

The CLEAR keyword causes the allocator to be cleared. All objects are removed from the allocator. However none of the keyword settings are changed. The size of the allocator may not be respecified after a CLEAR command.

The COPY keyword may be used to copy the data in an object in the allocator into a second object. The form of the command is

```
COPY fromname toname
```

where "fromname" must be the name of an object already in the allocator. If "toname" already exists in the allocator and is the same size as "fromname," the data in "fromname" will be copied into "toname." Otherwise "toname" will be created (or changed to have the correct size) and then the copy will occur. In all cases "fromname" is not changed. The COPY command may be used to "fool" Ptolemy into using a different potential or wavefunction in a subsequent part of the calculation.

The RENAME command is used to change the name of an object in the allocator. Its form is

```
RENAME oldname newname
```

where "oldname" must be the name of an object in the allocator. The name of this object will be changed to "newname." There must not be another object with the name "newname" already in the allocator; if there is, inconsistent results may occur.

The FREE command is used to delete an object from the allocator and thus make its space available for other objects. The command is followed by the name of the object to be freed. If the object does not exist, a warning will be printed and processing will continue with the next input line.

In the WRITENS, COPY, RENAME and FREE commands the first object name may be replaced with the actual number of the object in the allocator. However this practice is not recommended since it is difficult to predict the numbers of the objects.

An object may be added to or changed in the allocator by means of the ALLOCATE command. This command has the form

ALLOCATE name list-of-numbers

where "name" will be the name of the object in the allocator. The number of elements in the list-of-numbers determins the length of the object. The numbers may be in any format, with as many or as few as is desired per input line. If an object with the name "name" already exists, it is replaced with the new object as defined by the ALLOCATE command. In this manner one may read in arbitrary bound-state wavefunctions after Ptolemy has computed the bound-state wavefunctions for a Woods-Saxon potential. The new wavefunctions will then be used in a subsequent DWBA calculation.

The BIMULT keyword causes two objects (they may be the same object) to be multiplied together. The form of the command is

BIMULT name1 name2

where "name1" and "name2" are the names of the two arrays to be multiplied together. They must be of the same length. They will be multipied together in an element-by-element fashion and the resulting array will be stored in a new unnamed object in the allocator. Its number will be printed in the output. The numbers of the input arrays may be used inplace of their names.

The keyword NUMRNUM may be used to compute the matrix element between two wavefunctions of a power of r. The form of the command is

NUMRNUM name1 power name2

where "name1" and "name2" are the names (or numbers) of two objects in the allocator. They must be of the same length and must be wavefunctions that were computed with the present value of STEPSIZE. The integer "power" is the power of r that is to be included in the integral. The integral

Integral(0 to ASYMPTOPIA) dr r**power name1 name2

will be computed and printed.

The keyword NRNLIMS may be used to compute the partial matrix element of a power of r. The form of the command is

NRNLIMS name1 power name2 start stop

where "name1", "name2," and "power" are the same as for NUMRNUM. The range of the integral is specified by "start" and "stop" which are specified in fm.

The keyword PRINT may be used to control the amount of printing that Ptolemy does. It is followed by a five-digit integer that indicates the amount of printing that is to occur. Each digit controls different items of the printed output. The larger the digit, the more information that is printed. The default value is PRINT = 10001 which results in summaries of the input, the radial integral phases and magnitudes and the cross sections being printed. If the five-digit number is writen as PRINT = TMCXI, the significance of the digits is:

I = 0 - Only print the differential cross sections and final fit values.
1 - (Default) - Print summaries of input, magnitudes and phases of the radial integrals and elastic S-matrices in addition to output for PRINT=0. For fits the initial and final values are shown along with a summary of the path followed by the fitter.
2 - Print radial integrals as they are computed and give estimates of their cancellations. This option is strongly recommended as large cancellations are an indication that the convergence should be checked. The singular values are printed by the QUAVER fitter.
≥ 3 - Print debugging information.

X = 1 - The WKB amplitudes used to find the critical L are printed for each L.
2 - Debugging output is printed by the WKB routine.

C = 1 - Several lines are printed for every chi-squared function calculation made during the course of a fit. Debugging output from the Coulomb excitation integrals is printed. Work arrays are not freed following the radial integral computation.
2 - Convergence to the bound-state eigenvalue is printed.
4 - Debugging output from the L-interpolation is printed.

M = 1 - The elastic S-matrix element is printed every time a scattering wavefunction is computed.
4 - Debugging output is produced by the elastic wavefunction routine.

T = 1 - (Default) - Show conversion of FIT data to standard form.
4 - Some debugging output about the transfer effective interaction is produced.
9 - Enormous amounts of debugging output from the transfer effective interaction (the end has never been seen) are produced.

The value of PRINT may be changed at any time to effect subsequent printing except that in DWBA calculations the value of PRINT that was in effect at the time of the specification of the outgoing scattering state will determine the printing of the elastic S-matrices during the computation of the radial integrals.

IX - Acknowledgements

Much of the original development of Ptolemy was done by David Gloeckner. We wish to thank Frank Serduke for making available the subroutines that supply the data on nuclear charges, mass excesses, and spins. Larry Nazareth has been most helpful in giving us advance access to a number of subroutines that are being considered for inclusion in the Argonne Applied Mathematics Division MINPACK project. The Coulomb function subroutine is largly based on the Manchester subroutine RCWFN[+].

[+] A. R. Barnett, D. H. Feng, J. W. Steed and L. J. B. Goldfarb, Comp. Phys. Comm. <u>8</u>, 377 (1974).

Appendix A - List of all Keywords

The following lists contain brief descriptions and default values for all the Ptolemy keywords. Some of these keywords have not been discussed in the above text either because they are primarily designed for use in debugging Ptolemy or because it is doubtful that the average user will need them. They are all included here for completness. The entry "none" under "Default" means that the keyword is initially undefined. If it is not defined in the input and is necessary to the calculation, an error message will be printed and the job aborted. The entry "none*" under "Default" means that the keyword is initially undefined, but if it is not defined in the input, an appropriate value will be found by Ptolemy.

The keywords CROSSSECTION, GRIDSETUP, LINTERPOL, and RADIALINT are used inplace of the final semicolon to initiate individual stages of the DWBA calculation and should not be used in standard calculations. If desired the keywords DWBA or NZRDWBA may be used before the final semicolon to indicate that a DWBA calculation is to be done but they are not, at present, necessary.

All lengths are specified in fm and all energies are in MeV.

Reaction-defining Keywords

Keyword	Default	Meaning
BETA	none	Nuclear deformation parameter
BETACOULOMB	none	Coulomb deformation parameter
BELX	none	B(E,Lx,excitation)
E*i	0	Excitation energy in MeV of nucleus i (i = A, B, BIGA, BIGB, or X)
ECM	none	Incoming c.m. scattering energy in MeV
ELAB	none	Incoming Laboratory scattering energy in MeV
Ji	none	Intrinsic spin of nucleus i (i = A, B, BIGA, BIGB, or X)
Mi	none	Mass in AMU of nucleus i (i = A, B, BIGA, BIGB, or X)
MXCi	none	Total mass excess in MeV of nucleus i (i = A, B, BIGA, BIGB, or X)
MXCGi	none	Ground state mass excess in MeV of nucleus i (i = A, B, BIGA, BIGB, or X)
NUCONLY	off	Use only the nuclear part of the B.S. potential in the interaction potential
Q	none	Q-value in MeV
REACTION	none	Defines reaction in standard notation
SPAMP	1.	Projectile spectroscopic amplitude
SPAMT	1.	Target spectroscopic amplitude
SPFACP	1.	Projectile spectroscopic factor
SPFACT	1.	Target spectroscopic factor

Reaction-defining Keywords

Keyword	Default	Meaning
USECORE	on	Use Coulomb and real nuclear core corrections in the interaction potential
USECOULOMB	off	Use Coulomb with core corrections in the interaction potential
USEPROJECTILE	on	Use projectile B.S. potential as the interaction potential
USESIMPCOUL	off	Use Coulomb of just one B.S. in the interaction potential
USETARGET	off	Use target B.S. potential as the interaction potential
Zi	none	Charge of nucleus i (i = A, B, BIGA, BIGB, or X)

Two-body State Keywords

Keyword	Default	Meaning
A	none	Real W.S. diffuseness
AE	0	AE*Elab is added to A
AESQ	0	AESQ*Elab² is added to A
AI	none	Imaginary W.S. diffuseness
AIE	0	AIE*Elab is added to AI
AIESQ	0	AIESQ*Elab² is added to AI
ASI	none	Surface absorption diffuseness
ASO	none	Real spin-orbit diffuseness
ASOI	none	Imaginary spin orbit diffuseness
CHANNEL	none	Specifies a two-body channel.
E	none	Two-body c.m. energy in MeV (ELAB or ECM may be used in stand-alone or fits)
EINVERSE	off	Energy-dependant pots are in 1/ELAB
EPOWERS	on	Energy-dependant pots are in ELAB
E*P	none	Projectile excitation energy
E*T	none	Target excitation energy
J	none	Total two-body angular momentum
JP	none	Total projectile ang. mom. (for spin-orbit)
L	none	orbital angular momentum
M	none	Reduced mass in MeV/c**2
MP	none	Projectile mass in AMU
MT	none	Target mass in AMU
NODES	none	Number of bound state nodes for r > 0
R	none	Real W.S. radius
RO	none	Real W.S. radius parameter
ROE	0	ROE*Elab is added to RO
ROESQ	0	ROESQ*Elab² is added to RO
RC	none	Coulomb radius
RCO	none	Coulomb radius parameter
RCP	none	Coulomb radius of projectile

Two-body State Keywords

Keyword	Default	Meaning
RCT	none	Coulomb radius of target
RCOP	none	Coulomb radius parameter of projectile
RCOT	none	Coulomb radius parameter of target
RI	none	Imaginary W.S. radius
RIO	none	Imaginary W.S. radius parameter
RIOE	0	RIOE*Elab is added to RIO
RIOESQ	0	RIOESQ*Elab² is added to RIO
RSI	none	Surface absorption radius
RSIO	none	Surface absorption radius parameter
RSO	none	Real spin-orbit radius
RSOO	none	Real spin-orbit radius parameter
RSOI	none	Imaginary spin-orbit radius
RSOIO	none	Imaginary spin-orbit radius parameter
SP	none	Projectile spin
SPAM	none	Channel spectroscopic amplitude
ST	none	Target spin
TAU	0	Real S.O. depth relative to real W.S. depth
TAUI	0	Imag S.O. depth relative to imag W.S. depth
V	0	Real W.S. well depth
VE	0	VE*Elab is added to V
VESQ	0	VESQ*Elab² is added to V
VI	0	Imaginary W.S. well depth
VIE	0	VIE*Elab is added to VI
VIESQ	0	VIESQ*Elab² is added to VI
VSI	0	Surface absorption strength
VSO	0	Real S.O. well depth
VSOI	0	Imaginary S.O. well depth
ZP	none	Projectile charge
ZT	none	Target charge

Calculation Keywords

Keyword	Default	Meaning
ACCURACY	10^{-12}	Accuracy of bound state convergence
ANGLEMAX	90	Maximum scattering angle in degrees
ANGLEMIN	0	Minimum scattering angle in degrees
ANGLESTEP	1	Scattering angle increment in degrees
ASYMPTOPIA	20	Start of asymptotic region
COULOMBMULT	1.	Determins start of Belling expansion
DATA	–	Enters experimental data for a fit
DELTAVK	.05	Bound state search step size
DERIVSTEP	10^{-6}	Stepsize for numeric gradient of potentials
DWCUTOFF	10^{-3}	Minimum relative integrand to use in DWBA integral; minimum relative Coulomb amplitude for excitation
FITACCURACY	10^{-3}	Required relative accuracy of optical

Calculation Keywords

Keyword	Default	Meaning
		model parameter fit
FITMULTIPLE	500	Meaning depends on optical model fitter in use
FITRATIO	10^{-4}	Meaning depends on optical model fitter in use
GAMMADIF	5	DIF compression parameter
GAMMASUM	1	SUM compression parameter
INELASACC	10^{-5}	Required accuracy of Coulomb excitation
LBACK	none*	LMAX-LBACK is start of L-extrapolation
LMAX	none*	Maximum scattering partial wave L
LMAXADD	30	LMAX = Max(LMAXADD + Lcritical
LMAXMULT	1.6	LMAXMULT*Lcritical)
LMIN	none*	Minimum scattering partial wave L
LMINMULT	0.6	LMIN = Min(LMINMULT*Lcritical
LMINSUB	20	Lcritical - LMINSUB)
LOOKSTEP	250	Number of steps in grid-searching for PHI
LSTEP	1	Increment of L in radial integral computations In-between values are found by interpolation.
LX	none	Exchanged orbital angular momentum
MAPDIF	1	Gauss-point map type for DIF grid
MAPSUM	2	Gauss-point map type for SUM grid
MAXCOULITER	80	Max iterations for Belling's expansion
MAXFUNCTIONS	50	Maximum number of chi. sqr. computations allowed in an optical model fit
MAXITER	10	Max. number of iterations in bound state search
MAXLEXTRAP	100	Maximum allowed L-extrapolation
MIDMULT	2	SUMMID multiplier
NAITKEN	4	degree of interpolation polynomial
NBACK	4	Num. of backward steps in scattering wave asymptotic matching
NCOSINE	256	Size of fast-cosine table
NPCOULOMB	8	Num. points/cycle in Coulomb excitation
NPDIF	10	Num. of points in DIF grid
NPHIADD	4	Num. of steps to extend PHI grid
NPPHI	10	Num. of points in PHI grid
NPSUM	15	Num. of computed points in SUM grid
NUMRANDOM	0	Num. of random steps for some fitters
REINITIALIZ	0	Number of iterations between reinitialization of the fitter (mainly for POWELL65)
STEPSIZE	.1	Step size for solutions of two-body differential equations
STEPSPER	none	Number of steps per "wavelength" for solutions of two-body equations.
STEP1R	1	Starting value for scattering state dif. eqn.
STEP1I	1	Starting value for scattering state dif. eqn.
SUMMAX	none*	End of SUM grid

---

* A value will be computed by the program if one is not given by the user.

Calculation Keywords

Keyword	Default	Meaning
SUMMID	none*	Clustering point of SUM grid
SUMMIN	none*	Beginning of SUM grid
SUMPOINTS	6	Num. points/wavelength for SUM grid
VPOLYORDER	3	Order of interpolating poly for DIF grids

Control and Option-selecting Keywords

Keyword	Default	Meaning
ALLOCATE	-	Enter data into the allocator
BATCH	none*	Enter batch mode - an error terminates things
BIMULT	-	Multiply two arrays together
BOUNDSTATE	off	Stand-alone bound state is being entered
CHECKASYMP	off	Check approach of scattering state to asymptotic form
CLEAR	-	Clear allocator of all defined objects
CMANGLES	on	Angle grid is in c.m.
COMPLEXWAVE	on	Scattering waves have complex phase
COPY	-	Copy one object in the allocator into another
CROSSSECTION	off	Entering data for DWBA cross section stage
DAVIDON	off	Use the Davidon variable-metric fitter
DERIVCHECK	off	Check the analytic chi. sqr. gradients
DOASYMPT	on	Use Whittaker bound state asymptotic form
CALLTSO	-	Enter the TSO Command mode
DUMP	-	Print an object in the allocator
DUMPALL	-	The entire allocator is printed
DUMP2	-	Print an integer*2 object in the allocator
DWBA	-	DWBA input is being entered
ECHO	on	Input lines are printed in the output
ELASTIC	off	Compute cross section in stand-alone scattering
FIT	off	Do an optical model fit and specify the parameters to be varied
FITE	off	The bound state energy is matched to the potential
FITMODE	1	Meaning depends on optical model fitter in use
FITV	on	The depth of the real part of the W.S. well is matched to the bound state energy
FREE	-	Remove an object from the allocator
GRIDSETUP	off	Grid setup input is being entered
HEADER	-	Defines the header for subsequent pages
INCOMING	off	The incoming scattering state is being defined

---

* A value will be computed by the program if one is not given by the user.

Control and Option-selecting Keywords

Keyword	Default	Meaning
KEEP	-	Keep an object for subsequent Speakeasy use
KEYWORDS	-	List all keywords and their present values
LABANGLES	off	Angle grid is in laboratory
LINEAR	off	Only use linear extrapolation in the bound state search
LISTKEYS	-	List all keywords
LMCHOL	on	Use the LMCHOL sum-of-squares minimizer with
MINIM	off	Use the Fletcher variable-metric fitter
NEWPAGE	-	Go to new page for output
NOCHECKASYM	on	Do not check asymptotic form of scattering solution
NOECHO	off	Do not print input lines in the output
NOELASTIC	on	Do not compute cross sections in stand-alone scattering problems
NOSAVEB	on	Do not save B(Lx,MX,angle)
NOSAVEMXCROSS	on	Do not save (Lx,Mx) cross sections
NRNLIMS	-	Compute partial overlap of two functions
NSCATALOG	-	List names of all objects in allocator
NSDUMP	-	Print an object in the allocator
NSSTATUS	-	Print allocator statistics
NUMRNUM	-	Compute overlap of two functions
NZRDWBA	off	Input is for a nonzero-range DWBA
OUTGOING	off	Input is for the outgoing scattering state
PARAMETERSET	none	Specify a group of keyword definitions
POWELL65	off	Use the Powell 1965 sum-of-squares minimizer
PRINT	10001	Controls amount of printing
PRINTFIT	-	Print present E and V
PRINTWAV	-	Print last computed wavefunction
PROJECTILE	off	Projectile B.S. definition is being input
QUADRATIC	on	Use parabolic extrapolation in B.S. search
QUAVER	off	Use the QUAVER quasi-Newton fitter
RADIALINT	off	Input is for radial integration stage
REALWAVE	off	Real scattering waves for real pots.
RENAME	-	Change the name of an object in the allocator
RESET	-	Initialize for a new calculation - allocator is CLEARed and all keywords set to initial sta
RETURN	-	Terminate Ptolemy
ROCORD	off	Use the ROCORD generalized minimizer
SAVEHS	off	Form factor integrals will be saved
SAVEB	off	Save the B(Lx,Mx,angle) for KEEP
SAVEMXCROSS	off	Save (Lx,Mx) cross sections for KEEP
SCATTERING	off	Input is for stand-alone scattering
SIZE	-5000	Allocator size in bytes
SKIPASYMP	off	Do not use Whittaker function as asymptotic form of B.S. wavefunctions
TARGET	off	Input is for Target B.S.

Control and Option-selecting Keywords

Keyword	Default	Meaning
TSO	none*	Operating in interactive mode - errors allow corrections and retries
UNDEFINE	-	Set a keyword to undefined status
USEHS	off	Use previously computed form factor integrals
WRITENS	-	Write an object onto Fortran file 15
WRITESTEP	none	Interval (fm) at which wavefunctions are to be tabulated

Sub-keywords for DATA

The following are keywords that may appear within the paraentheses that follow the DATA keyword.

Keyword	Default	Meaning
ANGLE	-	C.m. angles of the data are being entered
ANGLESHIFT	0	Amount (in degrees) by which the angles are to be shifted in the laboratory frame
CHANNEL	-	Elastic channel of following data
CMANGLE	-	C.m. angles of data are being entered
CMSIGMA	-	C.m. cross sections in mb are being entered
ELAB	previous value	Laboratory energy of the data
ERROR	-	Errors have same units as data
LABANGLE	-	Lab. angles are being entered
LABSIGMA	-	Lab. cross sections in mb are being entered
MBERROR	-	Data errors are in millibarns
PERCENTERR	-	Data errors are in percent
POLARIZATION	-	Presently this data is ignored
RENORMALIZA	1	A quantity that will multiply each experimental cross section
SIGMA	-	Data is cross section in mb in ANGLE frame
SIGMATORUTH	-	Data is ratio of cross section to Rutherford cross section
WEIGHT	1	Each term in the chi-squared sum for the present data group is multiplied by WEIGHT

* A value will be computed by the program if one is not given by the user.

Appendix B - Core and CPU Time Estimates

Many Ptolemy calculations can be carried out in the Argonne Express class limits for the 370/195 of 250K and 2 minutes. However large calculations may exceed one or both of these limits and in such cases it is useful to be able to estimate the core and time requirements of the job. One method of so doing is to compare the "Peak Compressed Size" line with the "Allocator Size" line in the "Allocator Statistics" that are printed at the end of each job. The difference of these two numbers is the amount by which the REGION specified on the JOB card may be reduced in future runs of similar calculations. The Peak Compressed Sizes and CPU times from several jobs with varying conditions may also be used to estimate the needs of other calculations. Such rough estimates will almost always be adequate for optical model fits and inelastic excitation which are usually inexpensive jobs.

For large transfer calculations, one may want to use the following formidable formulas to estimate the job requirements. New users of Ptolemy should not be frightened by these formulas; they should simply ignore the rest of this section until they are forced to consider it.

The core size that should be given in the REGION parameter on the JOB card is determined by the size of the Ptolemy program and associated I/O buffers and by the Peak Compressed Size of the allocator. The first size is at present 90K. The second size is composed of a number of pieces, not all of which exist at the same time. The principal requirments (in double-precision words) are:

A. Scattering wave computations:

```
6*Max[SUMMAX, ASYMPTOPIA]/STEPSIZE + 10*(LMAX+Lxmax+1)
```

B. Scattering wave interpolations:

```
(Lxmax+3.5)*Npsum'*NPDIF
```

C. Computed radial integrals:

```
Num(Li,Lx) * (LMAX-LMIN+LSTEP)/LSTEP
```

D. Form-factor integrands:

```
NPSUM*NPDIF*(2*NPPHI+1)
```

E. Angular-transformation arrays:

```
(LMAX+Lxmax+1)/2 * { 9
  + Max[Lxmax + Max(LbndP, LbndT, Lxmax), LbndP+LbndT+1]
  + Num(Li,Lx)*(Lxmax+1)*[Min(LbndP, LbndT) + 1] }
```

F. Elastic S-matrix elements:

    4*(LMAX+Lxmax+1)

G. Elastic S-matrix elements for extrapolation:

    6*(Lmax'+Lxmax+1)

H. Interpolated and extrapolated radial integrals:

    4*(Lmax'-Lmin+1)*Num(Li,Lx)

I. Cross sections:

    Num(angles) * (4 + Lxmax-Lxmin)

In addition to keywords, the following symbols were used in the above:

```
Lxmax = Maximum Lx (transfered L);
Lxmin = Minimum Lx;
Lmax' = Maximum L for extrapolation;
LbndP = Projectile bound-state orbital angular momentum;
LbndT = Target bound-state orbital angular momentum;
Num(Li,Lx) = [ (Lxmax+Lxmin+2)(Lxmax-Lxmin+1) ]/2 ;
Npsum' = SUMPOINTS*(SUMMAX-SUMMIN)/[average wavelength] ;
Num(angles) = (ANGLEMAX-ANGLEMIN)/ANGLESTEP + 1 .
```

Using the above pieces, the allocator requirement for either a normal or a SAVEHS transfer calculation is estimated as:

    Max[A+B+C+D+E+F, F+G+H+I] + 500 ,

while for a USEHS calculation the estimate is:

    Max[A+B+C+F, F+G+H+I] + 500 .

In both cases the estimates are in double precision words; one should divide by 128 to convert to kilobytes (K).

The time estimate for a standard or SAVEHS run on the 370/195 is given in the following formula. Timings on other computers will be approximately proportional to this estimate. No estimate is given for USEHS runs since they are so fast.

$$\text{Time(seconds)} = 10^{-7} * \text{NPSUM*NPDIF*NPPHI} * [(\text{LMAX}^2 - \text{LMIN}^2)/\text{LSTEP}] * (\text{LbndP}+1)(\text{LbndT}+1) * \{ 1.9 + 0.68[(\text{Lxmax}+1)^2 - \text{Lxmin}^2] \}$$

This estimate refers only to the time involved in computing the radial integrals. The time for computing the scattering wavefunctions and the differential cross sections is usually negligible in comparison with this time.

Appendix C - JCL for Ptolemy Jobs

1. JCL at Argonne

Ptolemy runs that involve no KEEP, SAVEHS or USEHS commands may be made with the following JCL on Argonne's 370/195 or the CRC 370/165:

```
//jobname  JOB  (Fbadge,2,0,2),CLASS=C,REGION=250K
      account card
//  EXEC  PTOLEMY
      Ptolemy input
```

The above procedure defines FT06F001 as the output file, FT05F001 as the input, and STEPLIB as C109.PHYSICS.LOAD which contains the current production version of Ptolemy. For large calculations it may be necessary to modify the 2-minute time estimate or the 250K region estimate on the JOB card. The cost of small calculations can be slightly reduced by specifying a REGION of 200K or even 150K.

If a KEEP operation is to be made in a Ptolemy run, it is necessary to have a Speakeasy Keep dataset. This dataset must be a partitioned dataset with RECFM=FB, LRECL=80, and a reasonable block size such as BLKSIZE=1680. For ease in Speakeasy KEPT operations its name (at Argonne) should be Bnnnnn.SPEAKEZ.DATA where nnnnn is the user's badge number. Such a dataset is most easily made by logging on to TSO and using the ISPEAKEP command. Once the dataset has been made it will last indefinitely so one should not reuse the ISPEAKEP command for subsequent Ptolemy runs. Eventually the keep dataset will fill up so that from time to time it will be necessary to delete members and compress the dataset, or to make new keep datasets. When one has a keep dataset, it may be used in Ptolemy runs with the following JCL:

```
//jobname  JOB ... as above ...
      account card
//  EXEC  PTOLEMY
//MYKEEP  DD  DSN=Bnnnnn.SPEAKEZ.DATA,DISP=OLD
      Ptolemy input
```

The SAVEHS and USEHS commands use unformatted Fortran I/O. This requires a sequential dataset with the characteristics of RECFM=VBS,BLKSIZE=bbbb where bbbb is a reasonable size (3500 for 2314 drives or 4200 for 3330 drives). Ptolemy uses a special version of the Fortran I/O table that defaults to BLKSIZE=4200 so for 3330's it is not necessary to define BLKSIZE. Suitable JCL for a SAVEHS job is

```
//jobname  JOB ... as above ...
    account card
//  EXEC  PTOLEMY
//FT01F001 DD DSN=Cccc.Bnnnnn.somename,DISP=(NEW,CATLG),
//    UNIT=SHRT3330,SPACE=(TRK,(57,19),RLSE),DCB=RECFM=VBS
    Ptolemy input
```

This JCL will make a dataset that lasts one week; if it is anticipated that the dataset will be used for a longer time, UNIT=LONG3330 should be used. In the later case the dataset should be deleted when one is done with it. If KEEP operations are to be done in the same job, then the MYKEEP DD card should also be included (either before or after the FT01F001 DD card).

USEHS runs may be made with the following JCL:

```
//jobname  JOB ... as above ...
    account card
//  EXEC  PTOLEMY
//FT01F001 DD DSN=Cccc.Bnnnnn.somename,DISP=SHR
    Ptolemy input
```

Again the MYKEEP DD card should be included for KEEP operations.

From time to time, Ptolemy may be used in TSO at Argonne by entering the command

```
EXEC 'B88888.CMDPROC(PTOLEMY)'
```

or, if one is a B88888 system user, the command

```
PTOLEMY
```

may be used. If one intends to do KEEP operations in the TSO session, one should invoke Ptolemy with the following two commands:

```
ALLOC F(MYKEEP) DA(SPEAKEZ.DATA)
EXEC 'B88888.CMDPROC(PTOLEMY)'
```

Ptolemy makes very efficent use of the 370/195 CPU, and runs 10 to 17 times faster on the /195 than on the /75. Therefore anything but trivial Ptolemy calculations on TSO is strongly discouraged.

2. JCL at Other Installations

Other installations will not have the Ptolemy catalogued procedure used above. The following slightly lengthier invocation will therefore be needed:

```
//  EXEC  PGM=PTOLEMY
//STEPLIB  DD  DISP=SHR,DSN=name.of.ptolemy.load.dataset
//FT05F001 DD  DDNAME=SYSIN
```

```
//FT06F001 DD  SYSOUT=A,DCB=BLKSIZE=1596
(optional MYKEEP and/or FT01F001 DD cards)
  Ptolemy input
```

The BLKSIZE specified for FT06F001 is suitable for most installations that use ASP. However, at HASP sites it will probably be necessary to use BLKSIZE=133 (this must be specified; it is not the default). The optional MYKEEP and FT01F001 DD cards are written as in the above examples, except that local conventions for disk names, etc., will have to be used.

Appendix D - Sample Ptolemy Jobs

The following is the input for five sample Ptolemy jobs. These jobs use standard Ptolemy input sequences and, to reduce confusion, do not explore the alternative ways of defining a problem. The outputs of these examples are separately available from the authors of this report.

The following is an example of a five-parameter optical model fit to data at two energies. The depth of the real part of the potential is given an energy dependance while the rest of the potential parameters have no energy dependance. All of the potential radii will be equal to each other throughout the search while the real and imaginary diffusenesses will be separately varied. The search is first made with computed differential cross sections of moderate precision and is then repeated with more accurate values. Finally the differential cross sections for the two energies are printed on a uniform angular grid.

```
//EXAMPLE1 JOB (F12345,2,0,2),CLASS=C,REGION=200K,MSGLEVEL=(0,0)
     account card
// EXEC PTOLEMY
HEADER: EXAMPLE 1 - A TWO-ENERGY OPTICAL MODEL FIT
CHANNEL:  16O + 208PB
FIT ( RO=RIO=RCO  A  AI  V VE )
PARAMETERSET  EL1
RO = 1.3   A = .5  AI = .5  V = 40, VE = -.2    VI = 15
DATA  (  ELAB=104  ANGLE  SIGMATORU  PERCENTER
$   KOVAR ET.AL.   O16 ON PB208 AT 104 MEV
26.87        1.120      15.
32.21        0.994      5.
37.54        1.005      5.
42.84        1.006      5.
45.49        1.010      5.
48.13        1.000      10.
50.76        1.017      5.
53.39        1.020      10.
56.01        1.083      5.
58.62        1.170      5.
61.23        1.200      5.
63.83        1.120      10.
66.43        0.991      5.
69.01        0.790      10.
71.59        0.599      5.
74.16        0.432      15.
76.72        0.290      10.
79.27        0.209      10.
84.36        0.086      15.
89.40        0.038      10.
$   KOVAR ET.AL. O16 ON PB208 AT  $    ELAB = 140   WEIGHT = .3
 10.8        0.932      5.0
```

```
16.1        1.130    5.0
21.5        1.050    2.0
27.9        1.040    2.0
32.2        0.975    2.0
37.5        1.190    2.0
42.8        0.877    2.0
45.5        0.628    5.0
48.1        0.286    5.0
53.4        0.061    5.0
58.6        0.014    5.0
 )
 ;
PARAMETERSET EL2 ;
ELASTIC SCATTERING
ELAB = 104 ;
ELAB = 140 ;
RETURN
```

The second example is of inelastic excitation. The B(E2) value is used to determine both the Coulomb and nuclear deformation parameters. The optical potential in the incoming state will also be used in the outgoing state and for computing the effective interaction.

```
//EXAMPLE2 JOB (F12345,5,0,2),REGION=200K,CLASS=C
     account card
// EXEC PTOLEMY
HEADER: EXAMPLE 2 - INELASTIC EXCITATION
REACTION:    44CA(16O, 16O)44CA(2+ 1.156)    ELAB = 60
BELX = .0473
PARAMETERSET INELOCA1
INCOMING
V = 108  R0 = 1.207  A = .5074
VI = 21.2765  RI0 = 1.207  AI = .5192
RC0 = 1.2
;
OUTGOING
;
;  $  THIS FINAL SEMI-COLON STARTS THE DWBA
RETURN
```

The first transfer sample shows a calculation with no KEEP or SAVEHS, USEHS keywords. Note the use of PRINT=2 to cause the cancellations in the computed radial integrals to be printed. Although both bound states involve a spin-orbit force, it is not necessary to specify JP since it can be uniquly determined by Ptolemy from the other known spins and the given value of L.

```
//EXAMPLE3 JOB (F12345,2,0,2),CLASS=C,REGION=200K,MSGLEVEL=(0,0)
     account card
//   EXEC   PTOLEMY
HEADER:  EXAMPLE 3 - A SIMPLE TRANSFER CALCULATION
REACTION:   208PB(16O 15N)209BI(5/2- 2.84)     ELAB = 104
PARAMETERSET PB100A
PRINT = 2
PROJECTILE
NODES = 0   L = 1
R0 = 1.20  A=.65   RC0 = 1.20
VSO = 7
;
TARGET
NODES = 1   L = 3
R0 = 1.28   A=.76
VSO = 6   RSO0 = 1.09   ASO = .6
;
INCOMING
RC0 = 1.3   R0 = 1.2802  A = .5975  RI0 = 1.2962  AI = .5424
V = 20   VI = 15
;
OUTGOING ;
;  $  THIS FINAL SEMI-COLON STARTS THE DWBA
KEYWORDS
RETURN
```

In the following example we have both SAVEHS and KEEP commands. The Coulomb radius is not specified for the optical potentials, so a folded Coulomb potential from two uniform charge distributions will be used.

```
//EXAMPLE4 JOB (F12345,2,0,2),CLASS=C,REGION=220K,MSGLEVEL=(0,0)
     account card
//  EXEC  PTOLEMY
//MYKEEP   DD  DSN=B21541.SPEAKEZ.DATA,DISP=OLD
//FT01F001  DD  DSN=C109.PIEPER.EXAMPLE4,DISP=(NEW,CATLG),
//  UNIT=SHRT3330,SPACE=(TRK,(57,19),RLSE),DCB=RECFM=VBS
HEADER:  EXAMPLE 4 - TRANSFER WITH BOTH  SAVEHS  AND  KEEP
REACTION:    208PB(16O 15N)209BI(7/2- .90)  ELAB = 104
SAVEHS
PARAMETERSET PB100A
PRINT = 2
USECORE
PROJECTILE
NODES = 0    L = 1
R0 = 1.20  A=.65   RC0 = 1.25 ;
TARGET
NODES = 1    L = 3
R0 = 1.28   A=.76
TAU = .099558  ;
INCOMING
V = 50   VI = 50                                        $ FIT G, 104 MEV
R0 = 1.317   RI0 = 1.293   A = .419                     $ FIT G, 104 MEV
;
OUTGOING
;
ANGLEMIN = 30  ANGLEMAX = 120  ;
KEEP CROSSSEC FITG
RETURN
```

The final DWBA example is a USEHS run that refers to the output of the previous example. Here an energy-dependant optical potential is be used and thus the potential parameters in the outgoing channel will be slightly different from those in the incoming channel. Also RCO is now specified, so a point and uniform sphere Coulomb potential is used. The ANGLEMIN and ANGLEMAX specifications of the SAVEHS job will also be used in this job, but they could be changed here if desired. Note the small REGION size that may be used for USEHS's runs.

```
//EXAMPLE5 JOB (F12345,2,0,2),CLASS=C,REGION=170K
        account card
//  EXEC  PTOLEMY
//MYKEEP     DD  DSN=B21541.SPEAKEZ.DATA,DISP=OLD
//FT01F001   DD  DSN=C109.PIEPER.EXAMPLE4,DISP=SHR
HEADER:  EXAMPLE 5 - TRANSFER USING BOTH  USEHS  AND  KEEP
USEHS
$  NOTE ABSENCE OF REACTION, GRID AND BOUND STATE
$  DEFINITIONS.
INCOMING
V = 51.09   VI = 51.46                                    $ FIT B
R0 = 1.653   R0E = -.471E-2   R0ESQ = .109E-4             $ FIT B
A = -.651   AE = .01546   AESQ = -.4247E-4                $ FIT B
AI = -.629  AIE = .01416   AIESQ = -.369E-4               $ FIT B
RC0 = 1.3
;
OUTGOING
;
;
KEEP CROSSSEC FITB
RETURN
```

Distribution for ANL-76-11 Rev. 1

Internal:

B. Ancker-Johnson
G. T. Garvey
M. Peshkin
J. P. Schiffer
K. M. Pemble
R. J. Royston
S. C. Pieper (82)
ANL Contract File
ANL Libraries (5)
TIS Files (6)

External:

DOE-TIC, for distribution per UC-32 (203)
Manager, Chicago Operations Office
Chief, Chicago Patent Group
President, Argonne Universities Association
Physics Division Review Committee:
B. Bederson, New York U.
D. A. Bromley, Yale U.
W. L. Brown, Bell Telephone Labs.
R. Middleton, U. Pennsylvania
D. E. Nagle, Los Alamos Scientific Lab.
J. W. Negele, Massachusetts Inst. Technology
H. B. Willard, Case Western Reserve U.

☆ U.S. GOVERNMENT PRINTING OFFICE: 1977 750-133/33